

D360

Self-Service Data Access and Integration Benefits

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- **Certara is the fusion of 4 companies covering different areas of drug discovery & development**

- Tripos – Discovery
- Simcyp – Preclinical
- Pharsight – Clinical Data Modelling and Consulting
- Synchrogenix – Regulatory Writing



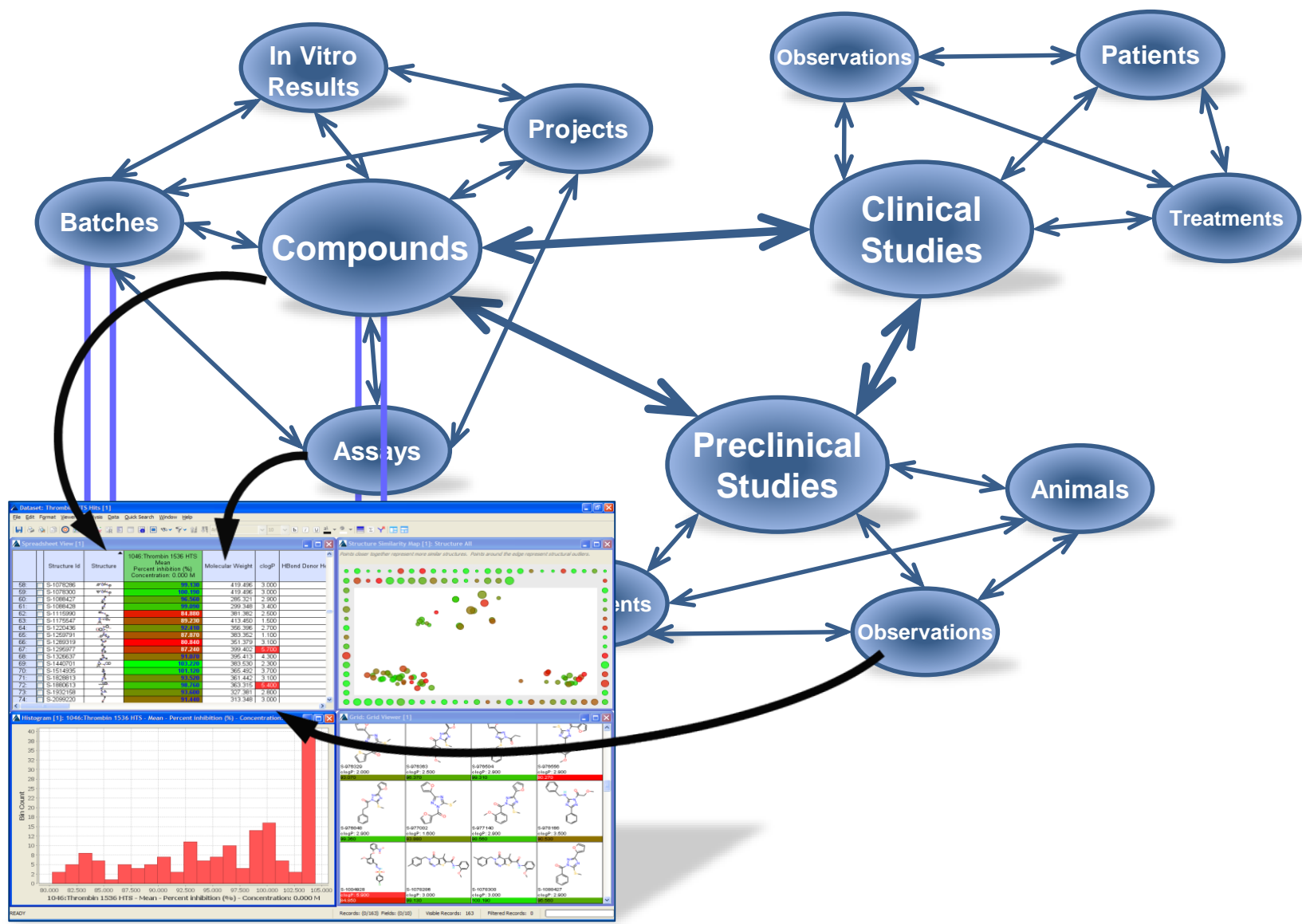
- **3 key areas of interest**

- *In Silico* modeling and prediction across discovery/development
 - Improved prediction of biological events from the molecular to the whole organism level
 - Leverage of technologies from formerly disparate areas
- Data access within and between expertise silos
 - Improved access to and thus use of data for all scientists throughout the process
 - Providing an ability to generate answers to a very wide range of scientific questions
- Integration of data access with modeling
 - Model creation for specific discovery and development end points
 - Model deployment throughout the discovery and development process

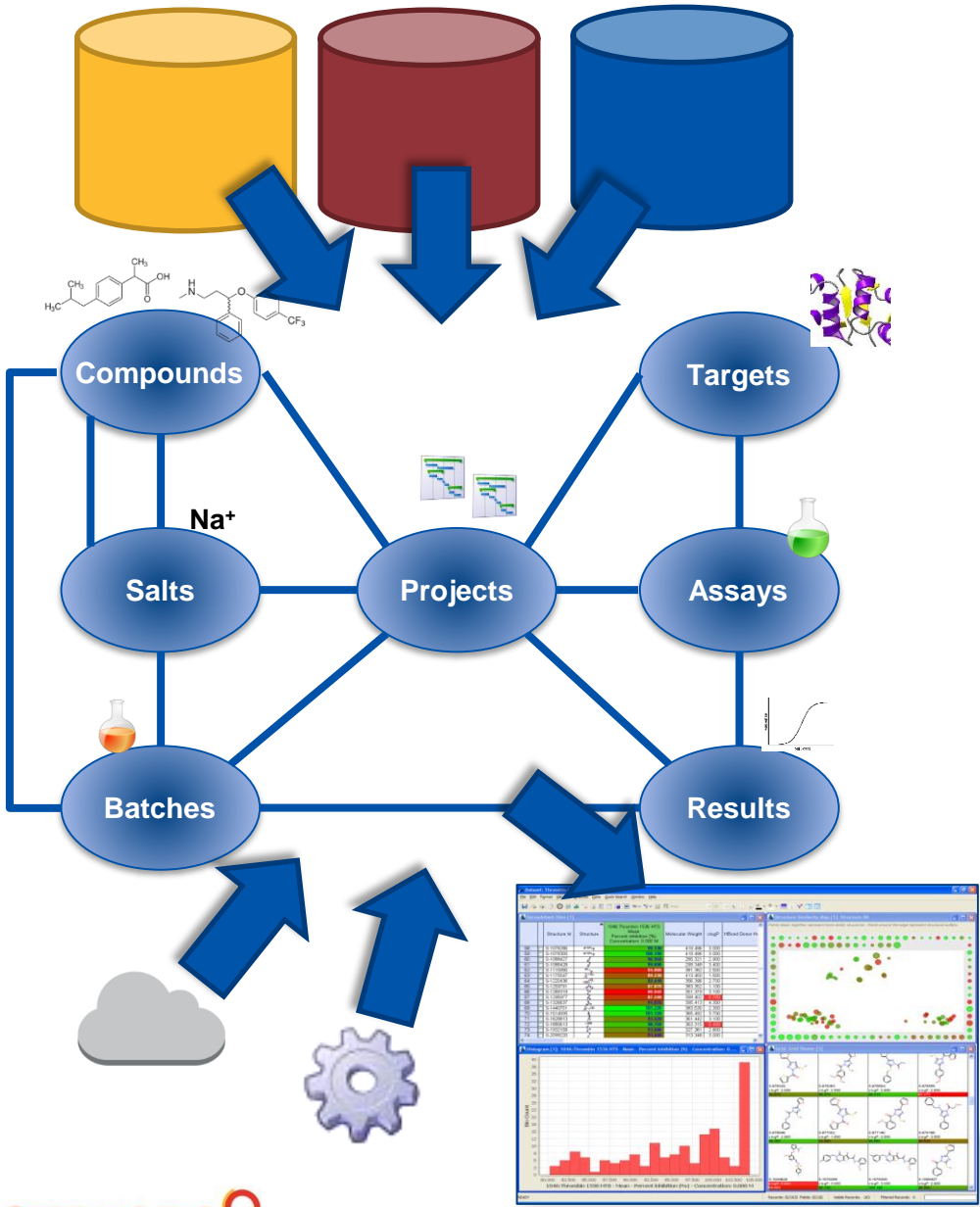
D360: A Self Service Data Analytics Tool

- **An application that supports research workflows:**
 - **Access** data (from multiple data sources)
 - **Analyse** data to gain insight
 - **Share** queries, datasets and information
- **D360 goals:**
 - Serve the needs of the scientist - workflows:
 - Provide an extensible, configurable discovery informatics platform
 - Allow data presentation from multiple aspects (Structure, Batch, Assay, Project, People...)
 - Reduce costs associated with maintenance of infrastructure
- **Application areas**
 - Drug Discovery
 - Standard project data views through complex data mining
 - Users from chemistry, biology, management...
 - ***Deployed to large and small organizations (Pfizer -> Agios)***
 - Preclinical
 - Animal PK/PD data
 - Safety Data – Tox/Path
 - Collaboration with Instem, Xybion, and others
 - ***Deployed to Toxicologists (AbbVie, Celgene...)***
 - Other
 - Clinical data informatics

D360: Physical vs Scientific Data Architecture



Benefits of a Scientific Data Architecture



- **Any Scientist can construct a data view**
 - Standard Project Data Views
 - Ad hoc data mining

- **Supports a wide variety of workflows:**
 - Standard Project data views
 - Exploratory SAR data mining
 - Assay QA/QC
 - Preclinical Study Monitoring
 - Cross study analysis

- **Supports informatics needs within and between scientific domains**
 - Discovery
 - Preclinical
 - Clinical

- **Frees up IT resources to perform higher value activities**

What does the user of D360 see?

- Any user of the system can build a data view
 - Without knowledge of specific data location/format
 - Without knowledge of Oracle, web services and other related technologies
 - And including data visualizations and analyses suitable for the task

The screenshot displays the D360 user interface, illustrating the process of building a data view and visualizing the results. On the left, a 'Choose Data Category' dialog box prompts the user to select a data category for their query. The 'Data Category' dropdown is set to 'Preclinical: Animals'. The main window shows a 'Query Animals Query [1]' with a list of fields to be included in the query, such as 'Study Number', 'Study Animal Number', 'Study Group Number', 'Animal Sex', 'Heart (Microscopic Observations) (HT)', and 'Weight (Terminal Body Weights)'. Below the field list, the 'Procedure Heart (Microscopic Observations) (HT)' is selected, and the 'Query Options' section is visible. On the right, a 'Spreadsheet View [1]' displays a table of query results with columns for 'Study Code', 'Study Animal Number', 'Animal Sex', 'Study Start Date', 'Heart Weight (g)', 'Terminal Study Weight (g)', and 'Study Duration'. Below the spreadsheet, a 'Histogram [1]' shows a distribution of 'Study Duration (days)' with a peak around 25-30 days. In the foreground, a scatter plot visualizes the relationship between 'Heart Weight (g)' on the x-axis and 'Terminal Study Weight (g)' on the y-axis. The plot shows a positive correlation, with data points colored by study duration and a red regression line indicating the trend.

Building a Self-Serving User Community

- Not Every user wants to build a query
 - D360 allows search capabilities to be Googled
 - Users who build data searches in D360 can “widgetise them”
 - Leverages the intellectual assets of the team

Thrombin Actives (Personal)

Percent inhibition (%) (1046, SD: Thrombin 1536 HTS):

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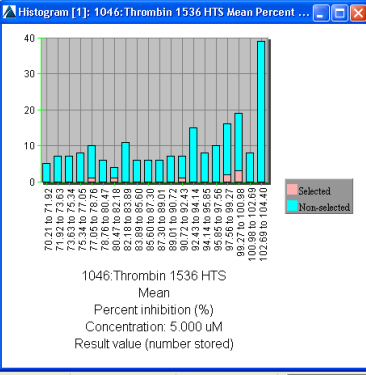
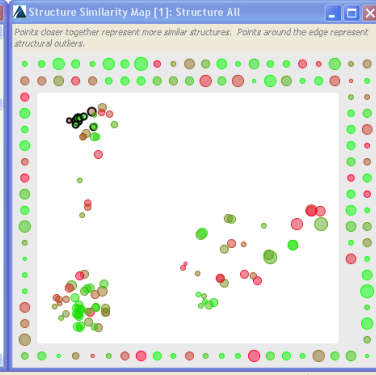
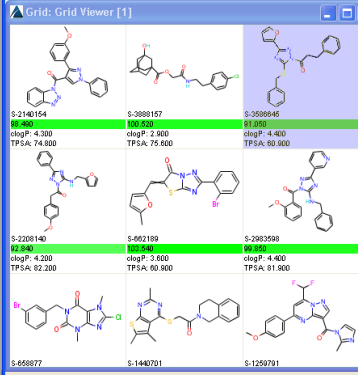
[Advanced](#) [Reset](#) [Open Containing Workspace](#)

Thrombin Actives

File Edit Format Viewers Analysis Data Help

Spreadsheet View [1]

	Main ID Number	Structure	1046:Thrombin 1536 HTS Mean Percent inhibition (%) Concentration: 5.000 uM	Molecular Weight	clogP	Acid pKa 1	Base pKa 1	HBond Donor Heteroatoms	HBond Acceptors	Rotatable Bonds	TPSA
59	S-5097725		100.000	372.463	5.700	3.921	3.192	1	4	4	59.300
60	S-995384		76.270	367.352	1.400	8.063	-2.886	0	7	4	65.100
61	S-5742239		82.500	366.453	3.100	11.790	25.286	0	4	7	42.000
62	S-1117440		76.560	366.437	3.400	13.846	19.374	1	4	5	76.900
63	S-3105236		100.000	366.371	3.100	18.732	9.016	1	5	4	105.000
64	S-1514935		69.720	365.492	3.700	6.595	-1.283	1	2	4	35.900
65	S-2177873		76.170	365.449	2.900	9.566	-10.855	0	2	4	43.900
66	S-3960319		95.340	365.429	4.000	21.242	5.298	1	6	7	81.900
67	S-5048498		96.750	365.386	3.700	16.260	-7.915	1	6	5	93.300
68	S-1880613		90.760	363.315	6.400	16.729	3.768	0	2	6	36.700
69	S-2600951		99.580	361.776	1.900	23.459	11.922	0	5	3	72.900
70	S-2300024		79.010	361.737	1.900	-0.440	-2.212	1	5	2	96.000
71	S-1828813		93.520	361.442	3.100	37.837	-1.745	0	6	6	81.000
72	S-2197230		86.360	361.417	4.400	19.456	19.796	0	4	5	60.900
73	S-3896375		75.130	358.393	4.300	7.966	19.919	1	5	6	73.000
74	S-650772		71.850	358.302	0.900	19.622	30.048	0	7	5	110.000
75	S-16189092		94.070	357.427	3.400	14.315	22.539	0	5	7	68.500
76	S-1220436		92.410	356.396	2.700	13.816	4.451	0	5	3	62.600
77	S-647714		81.030	354.449	2.600	2.142	-11.643	1	6	4	75.900
78	S-2973644		70.960	354.378	4.100	1.827	14.862	1	6	6	69.000
79	S-2110195		92.100	353.200	5.200	15.769	12.314	1	6	6	61.200



D360 Integration and ChemAxon

- **Technical resources can add greater value through integration**
 - D360 supplies an SDK and public APIs for both the client and server sides for scripting and code development
 - Used to integrate
 - Logistics and Productivity Tools
 - Calculation Engines
 - New Data sources
 - New Analysis capabilities
- **Support for ChemAxon tools has been key for Certara and D360 customers**
 - Support for chemistry search
 - JChem Cartridge and Web Services
 - Compound Registration
 - Integration with ChemAxon tools on the desktop:
 - Marvin
 - JChem for Excel
 - Calculate data using property calculators
- **We are very excited about integrating the new biologics tools from ChemAxon**

