CERTARA
Implementing Translational Science

D360
Self-Service Data Access and Integration Benefits

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Tripos SIMCYP Pharsight

- **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

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D360: A Self Service Data AnalyticsTool

- **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

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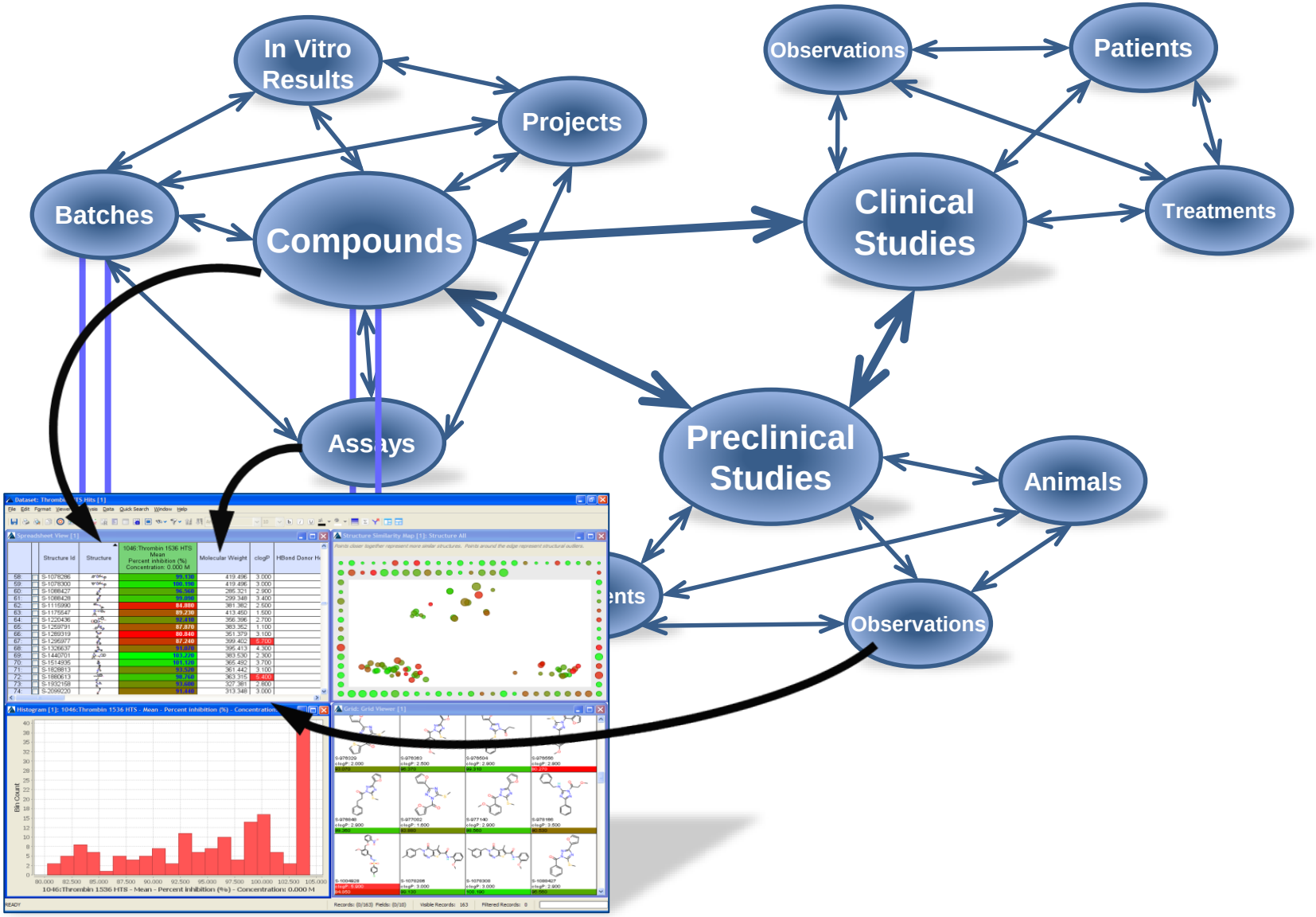
D360: Physical *vs* Scientific Data Architecture



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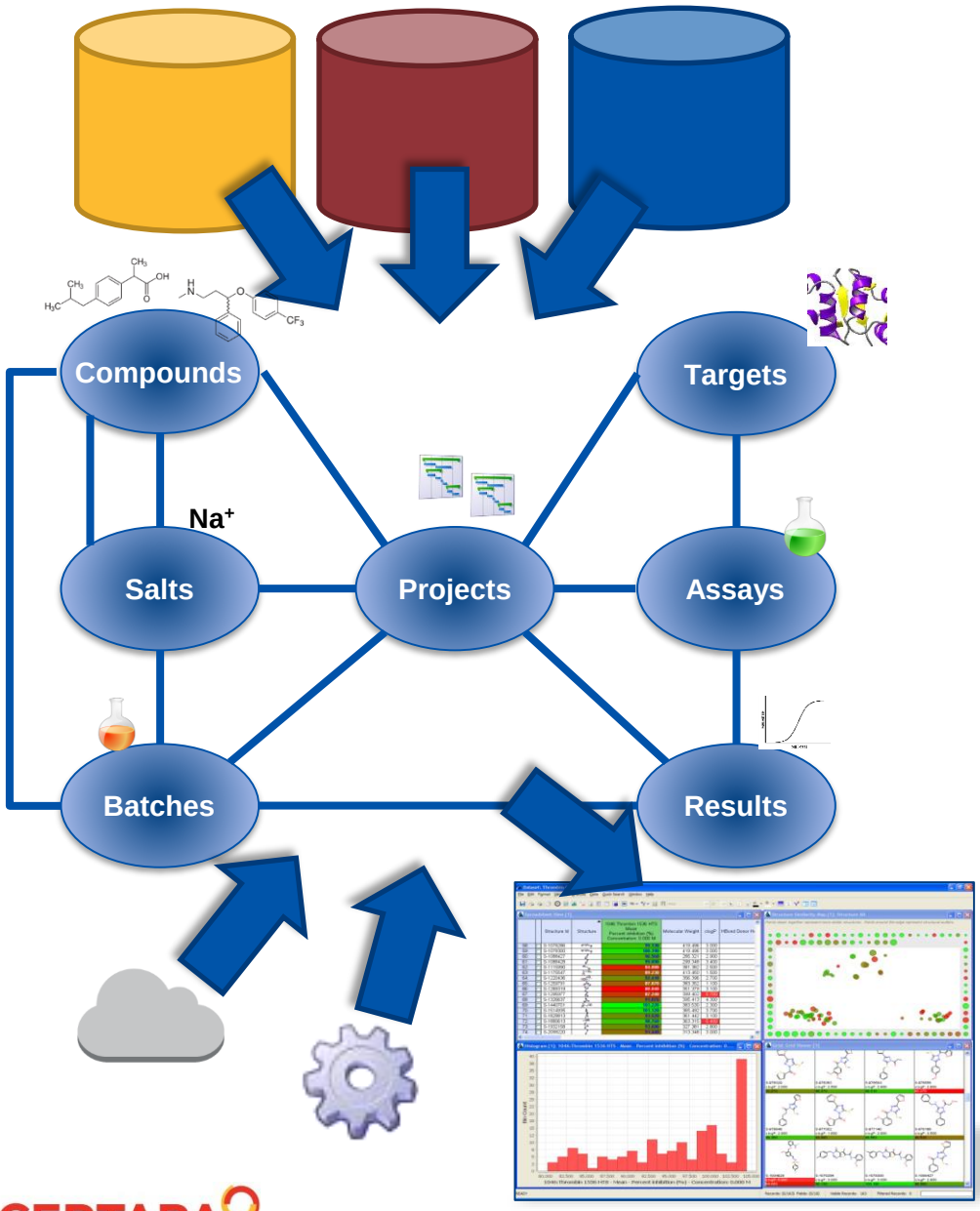
Benefits of a Scientific Data Architecture



- **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**

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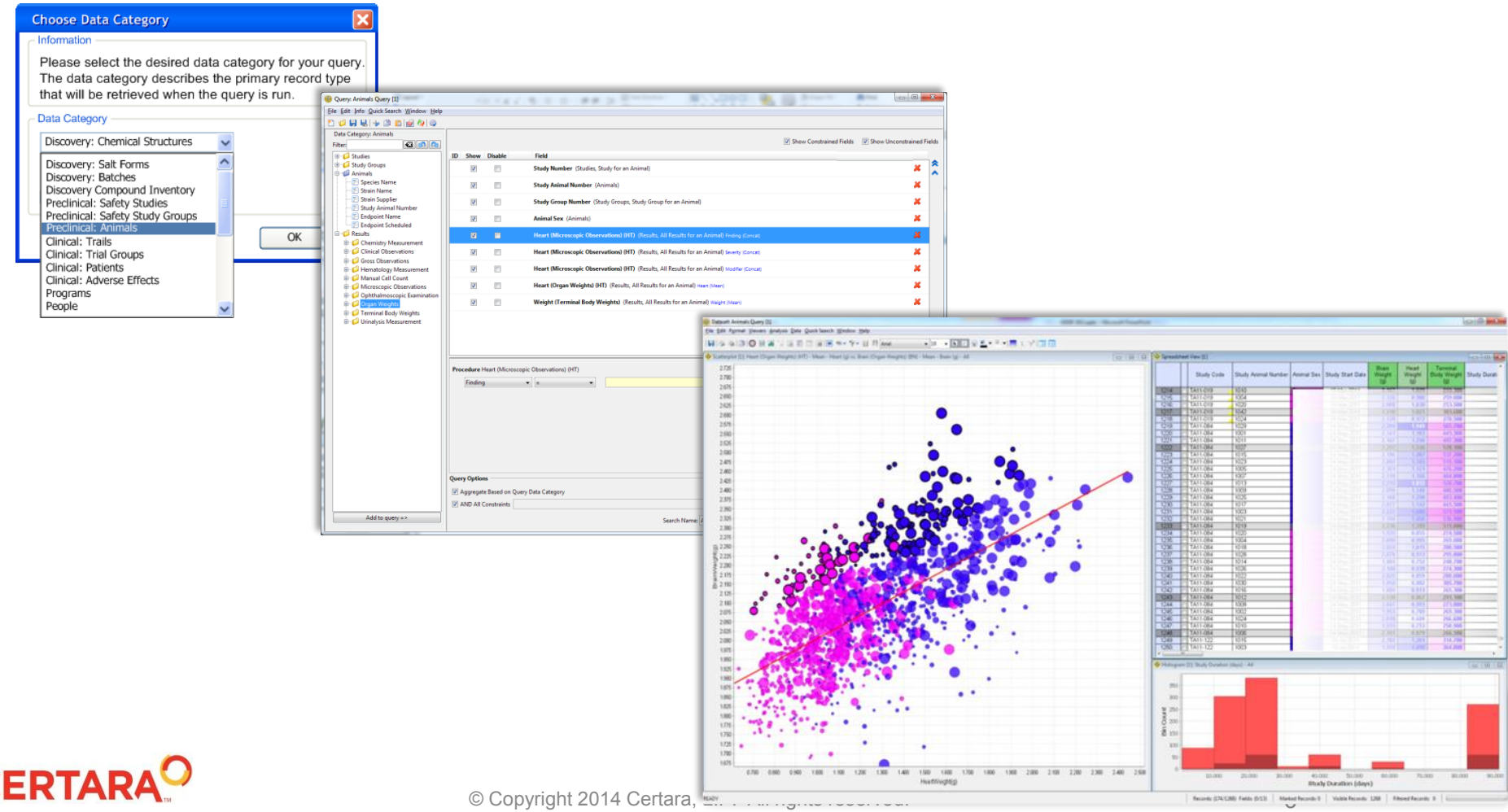
What does the user of D360 see?

- **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



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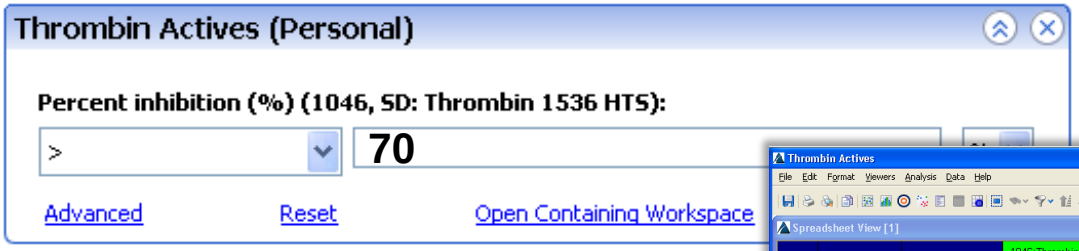
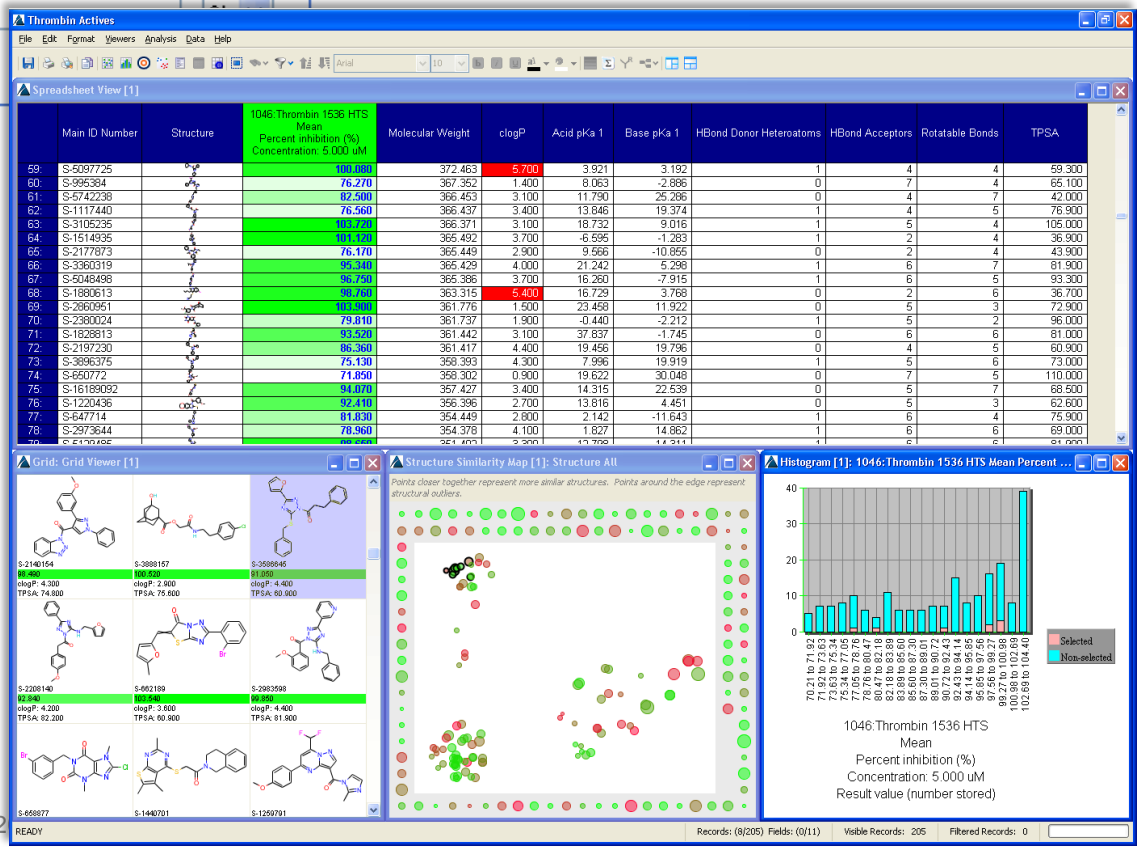
Building a Self-Serving User Community

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





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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**

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