

ChemAxon User Group Meeting, Budapest 2011

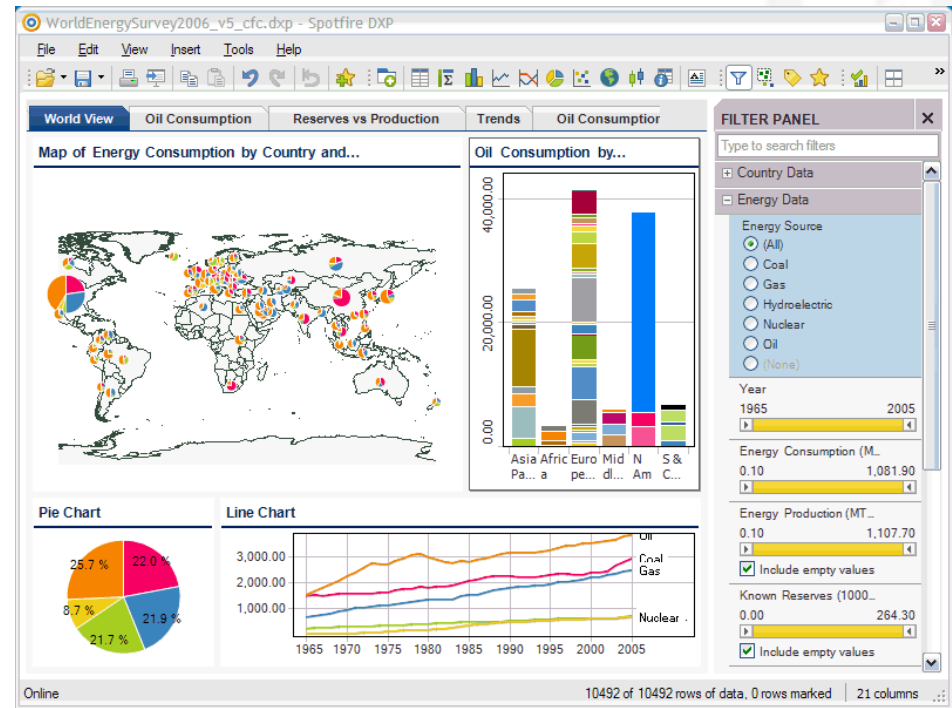
High Speed SAR Analysis with TIBCO Spotfire

Dr. Christof Gänzler, Sr Solutions Consultant

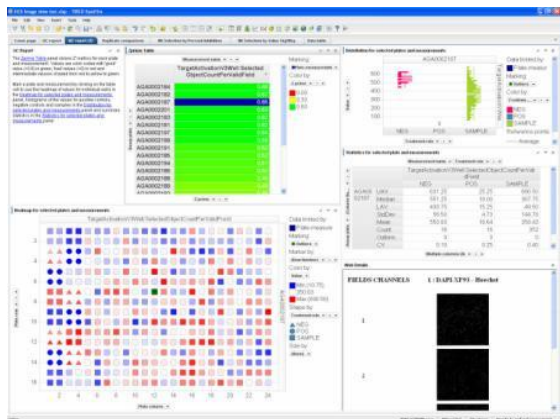


What is Spotfire?

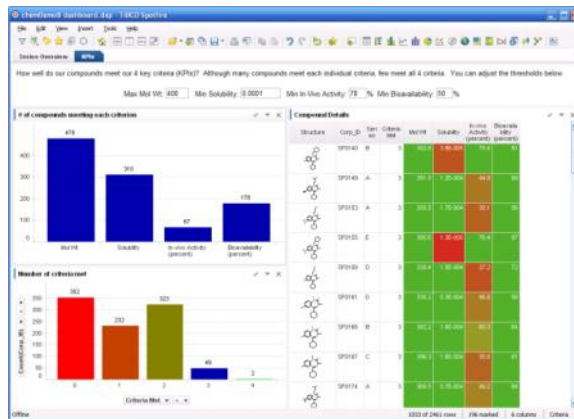
- Unique interactive visual analytics to spot trends, outliers and other hidden relationships in data
- Applicable to many different types of data
- Easily accesses data from multiple, disparate sources (Oracle, Excel, SAP, etc.)
- Helps deploy best practices
- Extensible platform with an open SDK



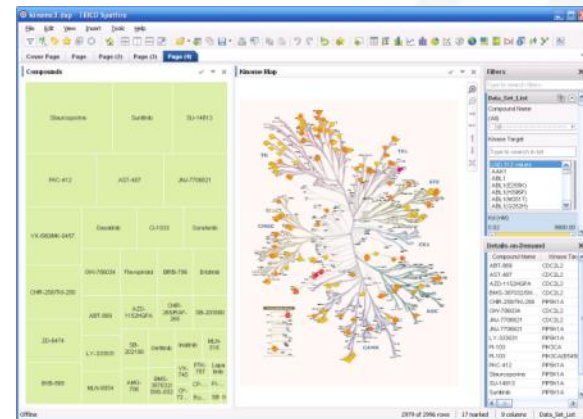
TIBCO Spotfire: One Platform, Many Applications



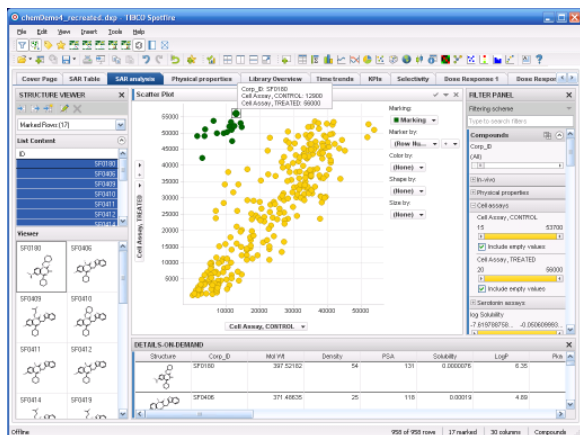
HCS, HTS



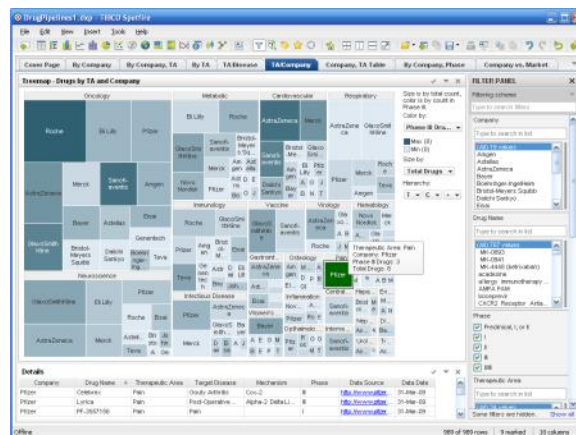
Project KPIs



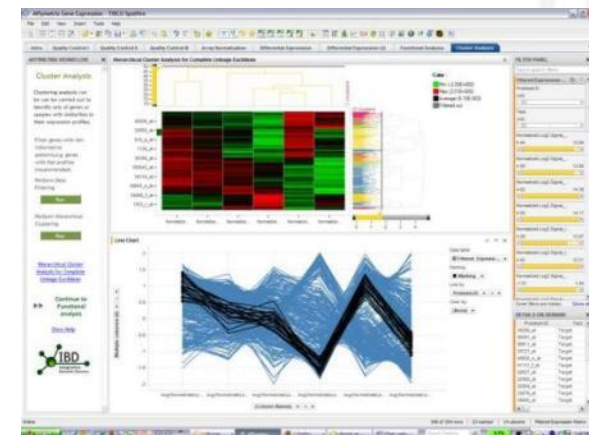
Kinase Inhibitors



SAR

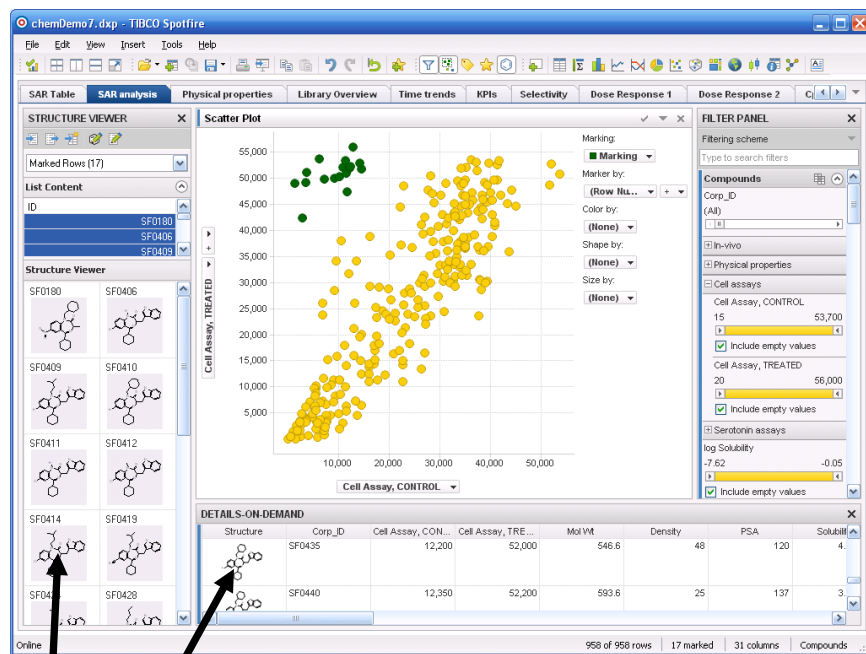


Competitive Intelligence




Gene Expression


Spotfire Integration with ChemAxon



Spotfire Client

 MarvinView

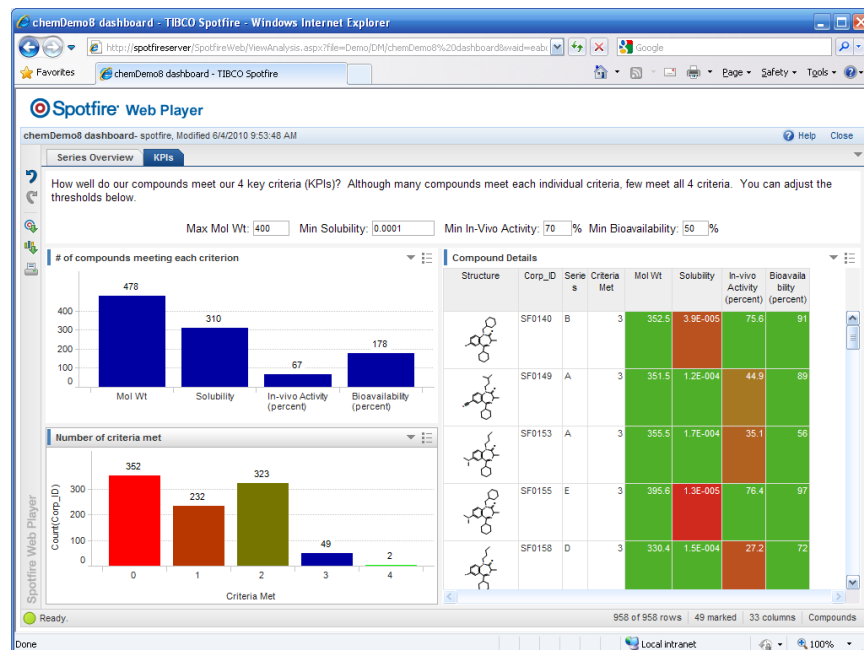

Spotfire Server


JChem Cartridge

Chemistry Project Dashboard

For: Team Leaders, Project Managers, Scientific Management

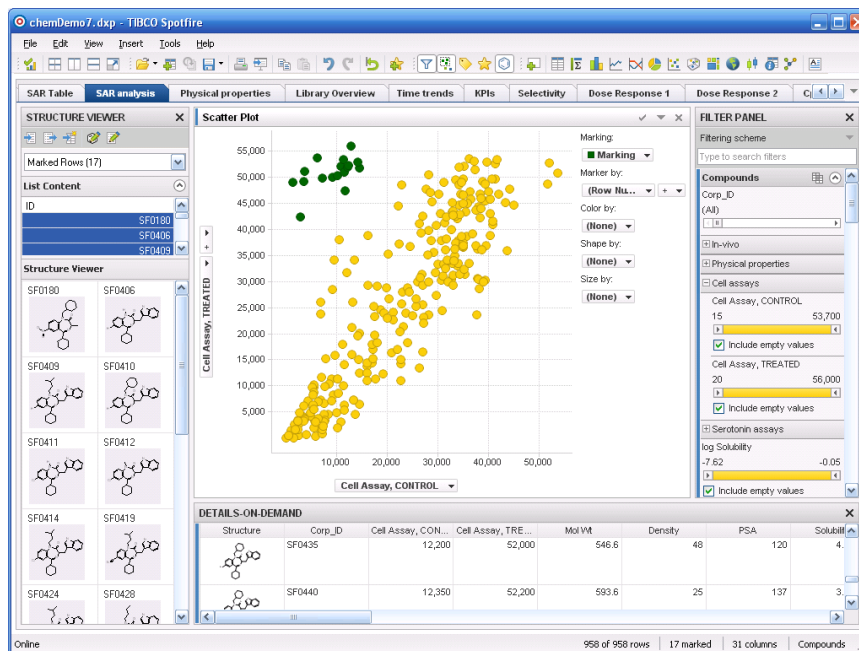
- How is my project doing vs. goals?
- Which series looks most promising?



SAR

For: Medicinal Chemists, Computational Chemists, Biologists

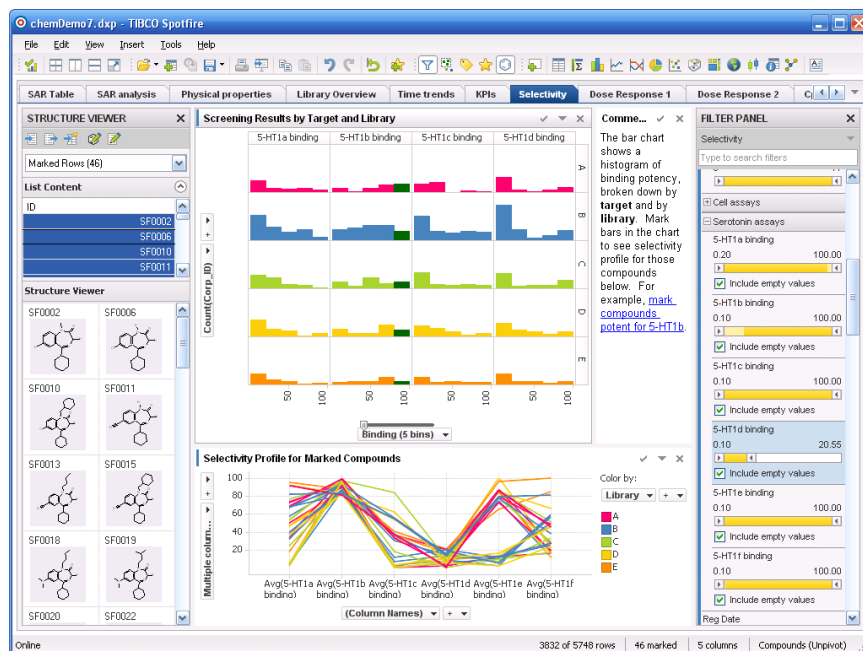
- Are there trends? Outliers?
- What's the structural basis for observed activity?
- What should I make next?



Selectivity Analysis

For: Screening Biologists, Lead Chemists

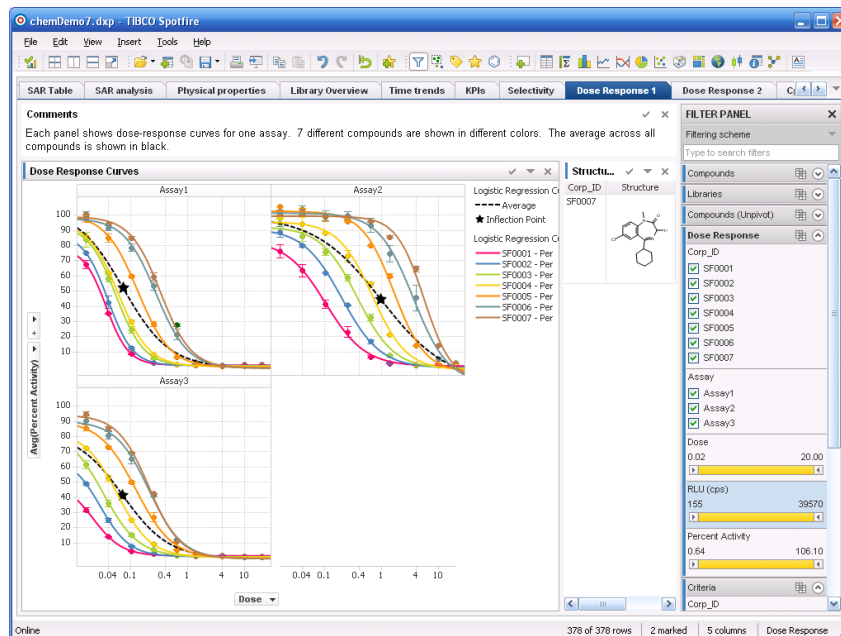
- How do my compounds behave across targets?
- Which compounds are selective, and why?
- Which compounds should advance?



Dose Response

For: Screening Biologists, Team Chemists

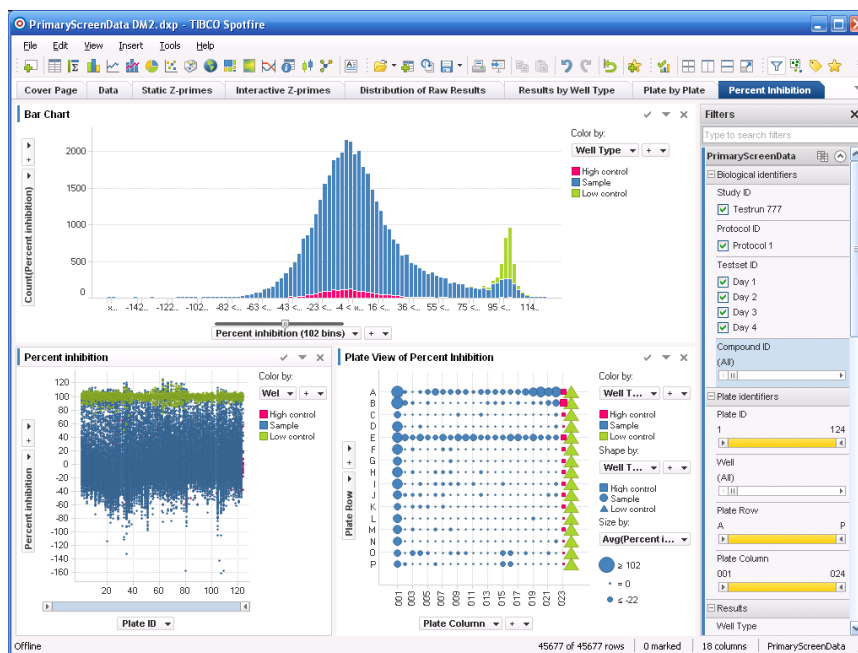
- How do my lead compounds behave in different assays?
- How do my lead compounds compare to a reference compound?
- How reliable are my IC50 values?



High Throughput Screening

For: Screening Biologists, Team Chemists, Team Biologists

- How do I detect systematic quality issues?
- How do I identify hits?



Competitive Analysis

For: Researchers, Managers

- Where is my company strong and weak?
- What therapeutic areas, diseases, mechanisms are best to target?

