



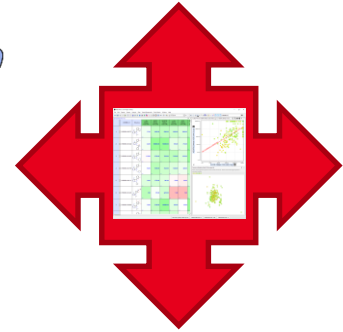
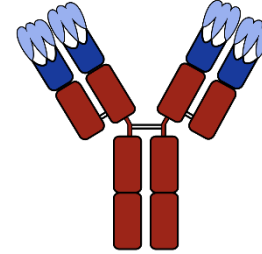


Evening Activity: Meet at the hotel lobby @ 5.30pm – Bus leaves at 6.00pm

UGM Goals

- A chance to Learn from the experience of others

- Pre-competitively
- About D360 utilization
- About informatics challenges



- A chance to guide strategic product direction

- Top 3 questionnaire
- Input to the D360 customer steering committee



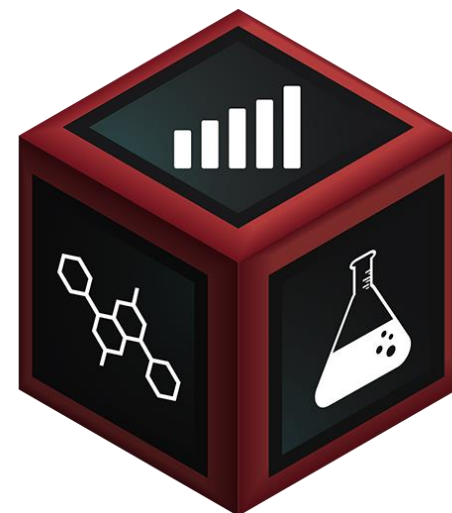
- A chance to drive best practices

- Data Analysis for pharmaceutical research
- Research Workflows
- Data architecture
- Collaboration



Certara's D360 People in the Room

- Thomas Kerbusch
 - Responsible for the Certara Consulting and Software Business
- D360 Development Team
 - Scott Seaton: D360 Core Development team
 - Dale Neely: Principal Developer
 - Doug Webster: Principal Developer
- D360 Services Team
 - Dennis Powell: Senior Scientific Consultant
 - Fabian Rauscher: Senior Informatics Consultant
 - Ian Ingram: Enterprise Informatics Consultant
 - Jason Burbank: Enterprise Informatics Consultant
 - Aaron Hohos: Enterprise Informatics Consultant
- D360 Business Development and Marketing:
 - Mannix Aklian
 - Shawn Hasan
 - Bradley Snipes
 - Kristine Christie



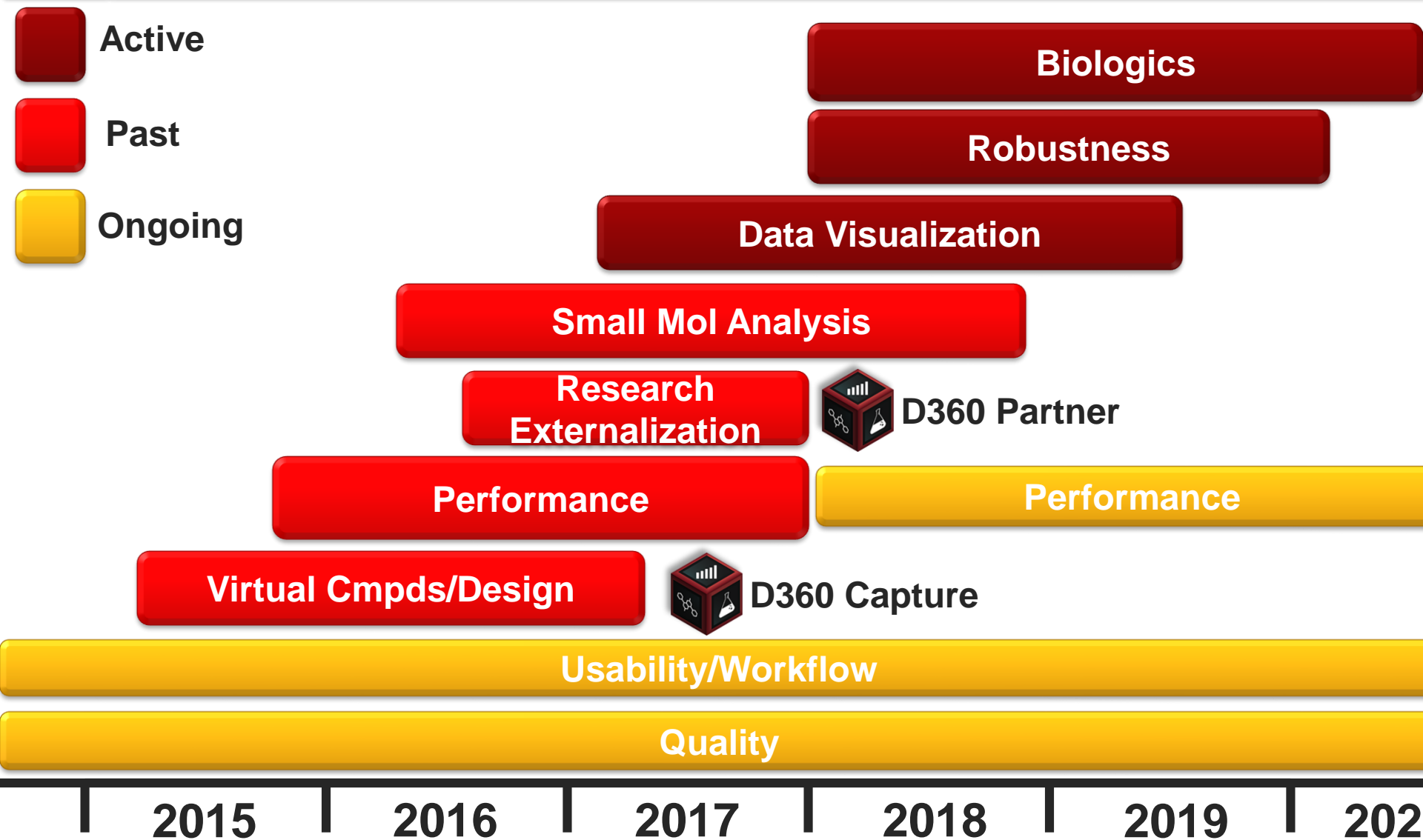
CERTARATM

Recent D360 Magic

D. R. Lowis D. Phil.



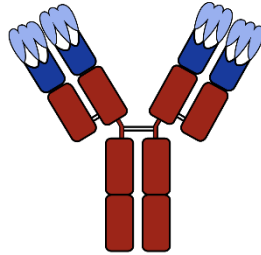
D360 Product Development Themes



Meeting Themes

- **Biologics:**

- Roche
- Regeneron
- Certara



- **Deployment and Configuration:**

- Arvinas
- Certara (x2)



- **Data Workflows:**

- Merck KGaA
- AstraZeneca (x2)
- Eisai
- Pfizer
- Certara



Sources for D360 Development

- D360 Customer Steering Committee
 - Provides strategic direction for the product

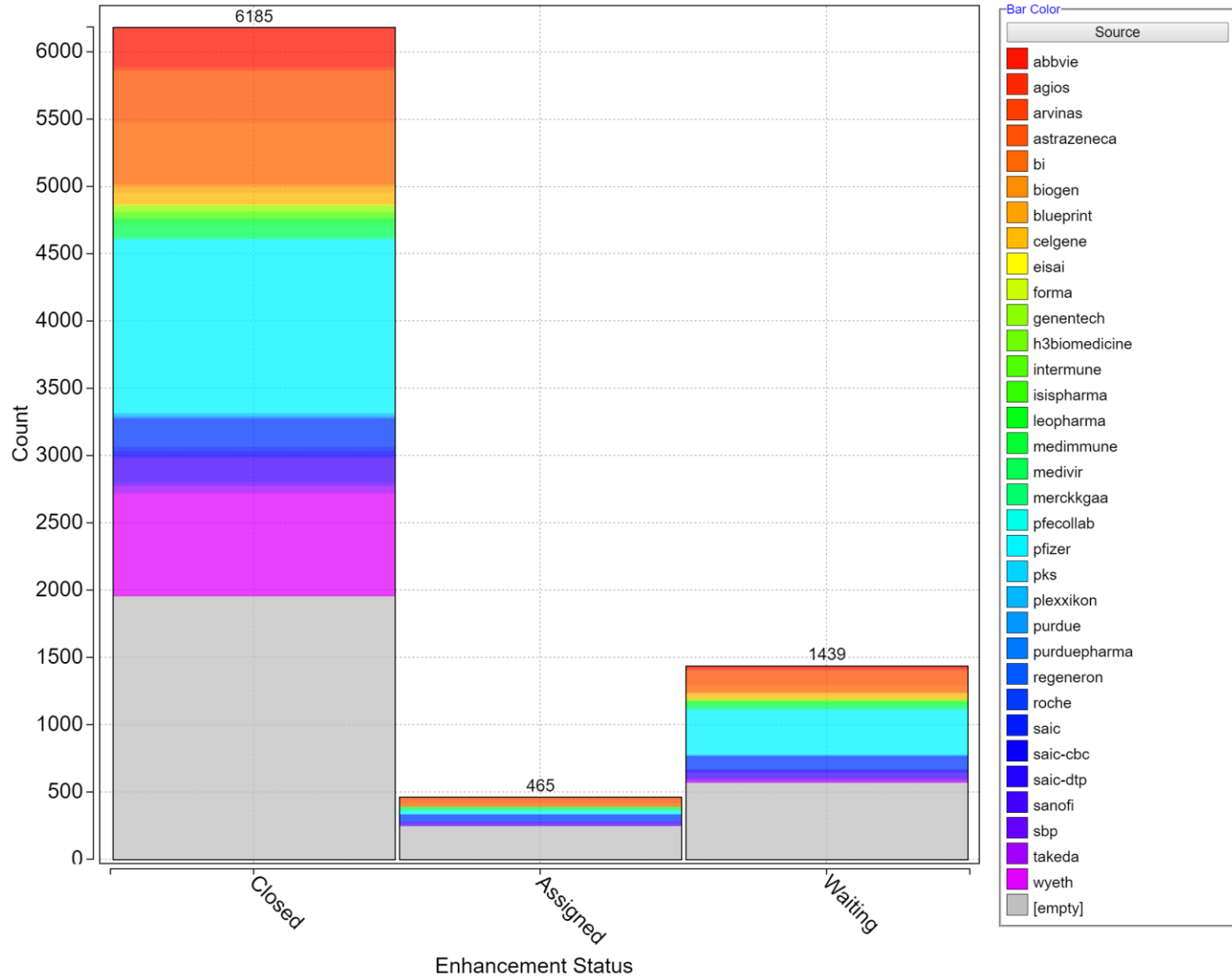
D360 Customer Steering Committee Priorities

1. D360 data source robustness
2. Automated testing – more robust testing
3. Logging and Monitoring
4. Biologics
5. Biology workflows – curve rendering
6. Web AED/Display of dataset in web
7. Improved workflows

Sources for D360 Development

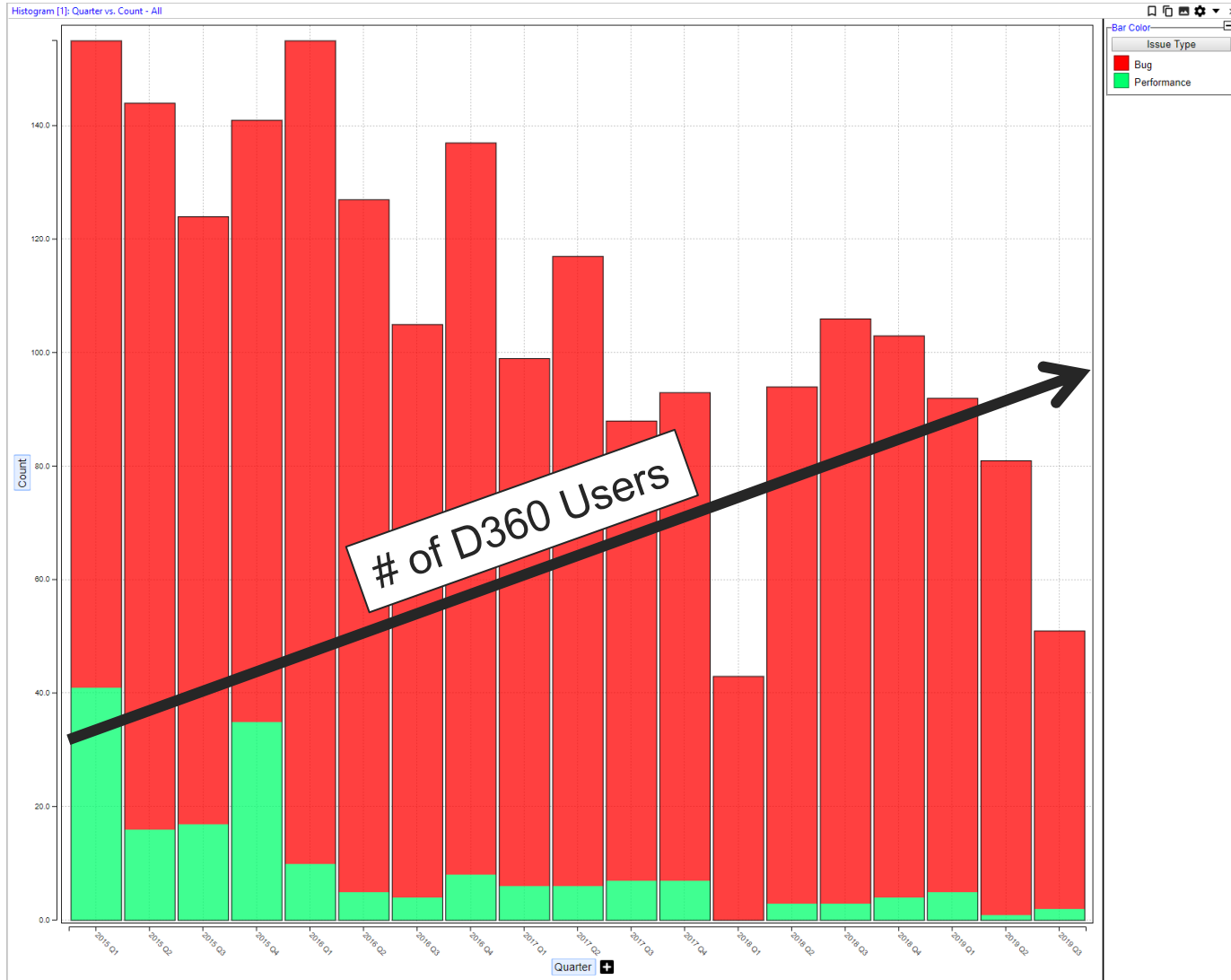
- User Input: Direct via D360 & through conversation

8098 Filed Enhancement Requests



What about Quality...

- Issues filed by end users



Recent (19.x) and Upcoming (20.1) D360 Releases

- Two D360 Releases per year:

February 31st and June 30th

- Many significant improvements:

- Biologics
- Data Visualization
- Scientific Enhancements
- Workflow (Usability)
- Deployment

- One of the key differentiators of D360 – attention to

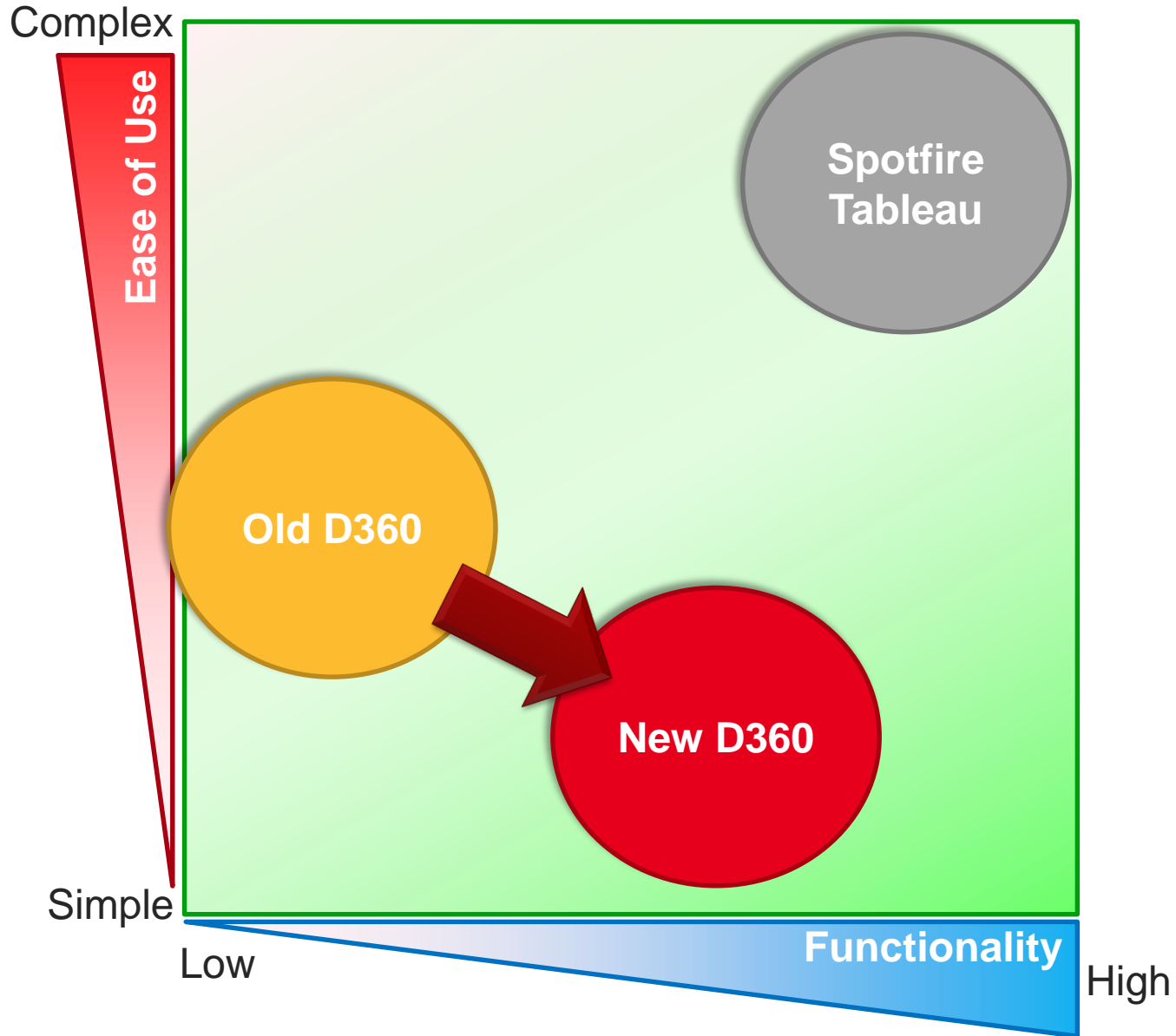
- Scientific data needs special treatment
- Working closely with customers is key

It's clear that you've worked with scientists to develop D360



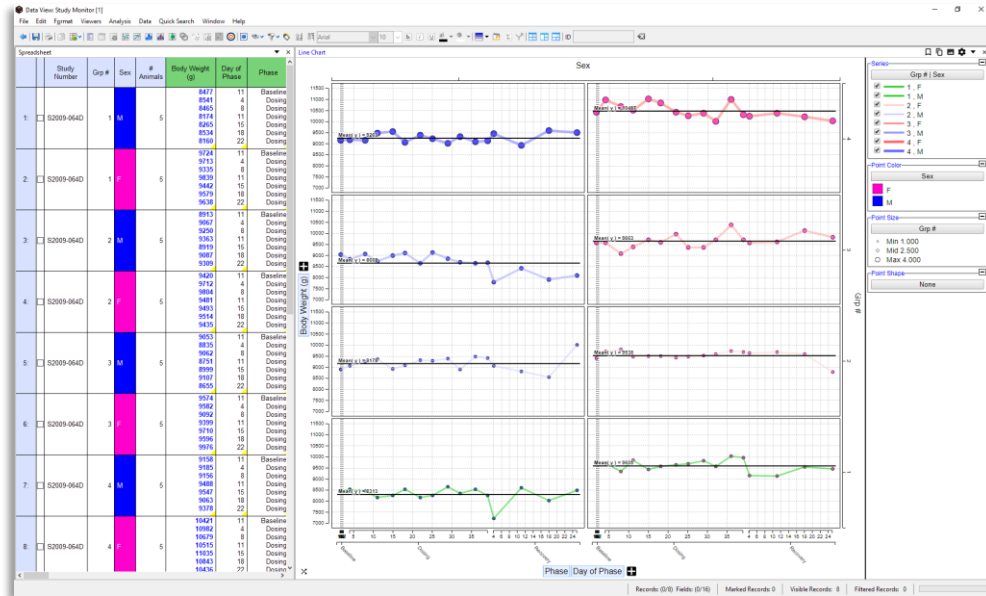
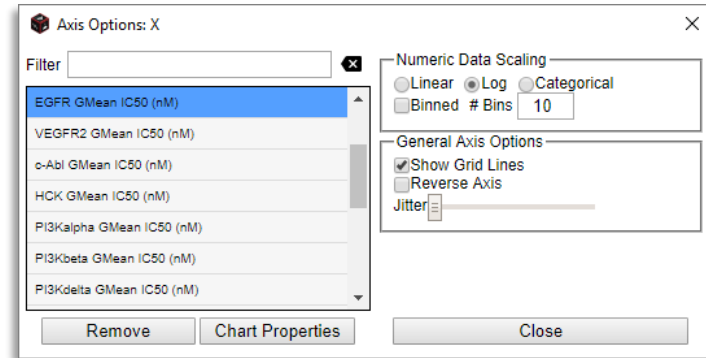
**Thank
You!!!**

Data Visualization: The Target



Key Design Features: All D360 Charts

- Simple to use:
 - Simple axis options for common changes
 - Easy axis flip
 - Chart duplication
- The right level of functionality
 - User defined lines
 - Trellising
 - Selection from the Legend
 - ...
- Attention to Scientific Detail
 - Linear/Log scaled axes
 - Structures on axes
 - Categorical axis ordering
 - Handles multi-value per cell data



Data Visualization: Dose Response Curves

ChEMBL Id

Structure

Inhibition of recombinant c-Src by radioactive phosphotransfer assay in presence of 10 pIC50 (Mean)

Inhibition of recombinant c-Src by radioactive phosphotransfer assay in presence of 10

Retrieve everything tested Retrieve everything tested from: Last N Days

Results & Conditions Analysis Information

Results

- IC50 (uM) (GMean)
- IC50CURVE
- pIC50
- Asymptote Maximum (%)
- Asymptote Minimum (%)
- Slope
- % Effect (%)

Curve Options

Axis Ranges

X-Axis: Min 1E-12 Max 1E-4

Y-Axis: Min 0 Max 120

Multi Curve Single Curve

Multi-Curve Color Scheme Rainbow Scheme Start Color Blue End Color Red

Dose Response Curve Show Line Thickness 2 Line Style Solid

Asymptotes (Min/Max) Show Line Thickness 1 Line Style Dashed

Result Line Show Line Thickness 1 Line Style Solid

XY Data (Dose-Response Points) Show

Included Values Point Shape Circle Point Size 3

Excluded Values Point Shape Inverted Triangle Point Size 3

Legend

Show Legend LOC_RIGHT

Available Data Fields:

Experiment Comment

Bioloist

Displayed Data Fields:

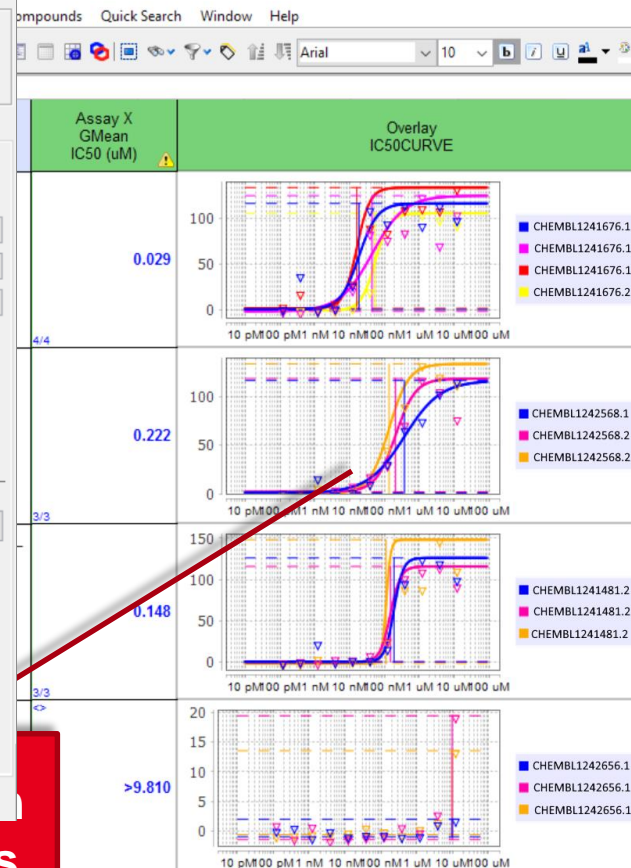
Batch Tested

Date Tested

Add >

< Remove

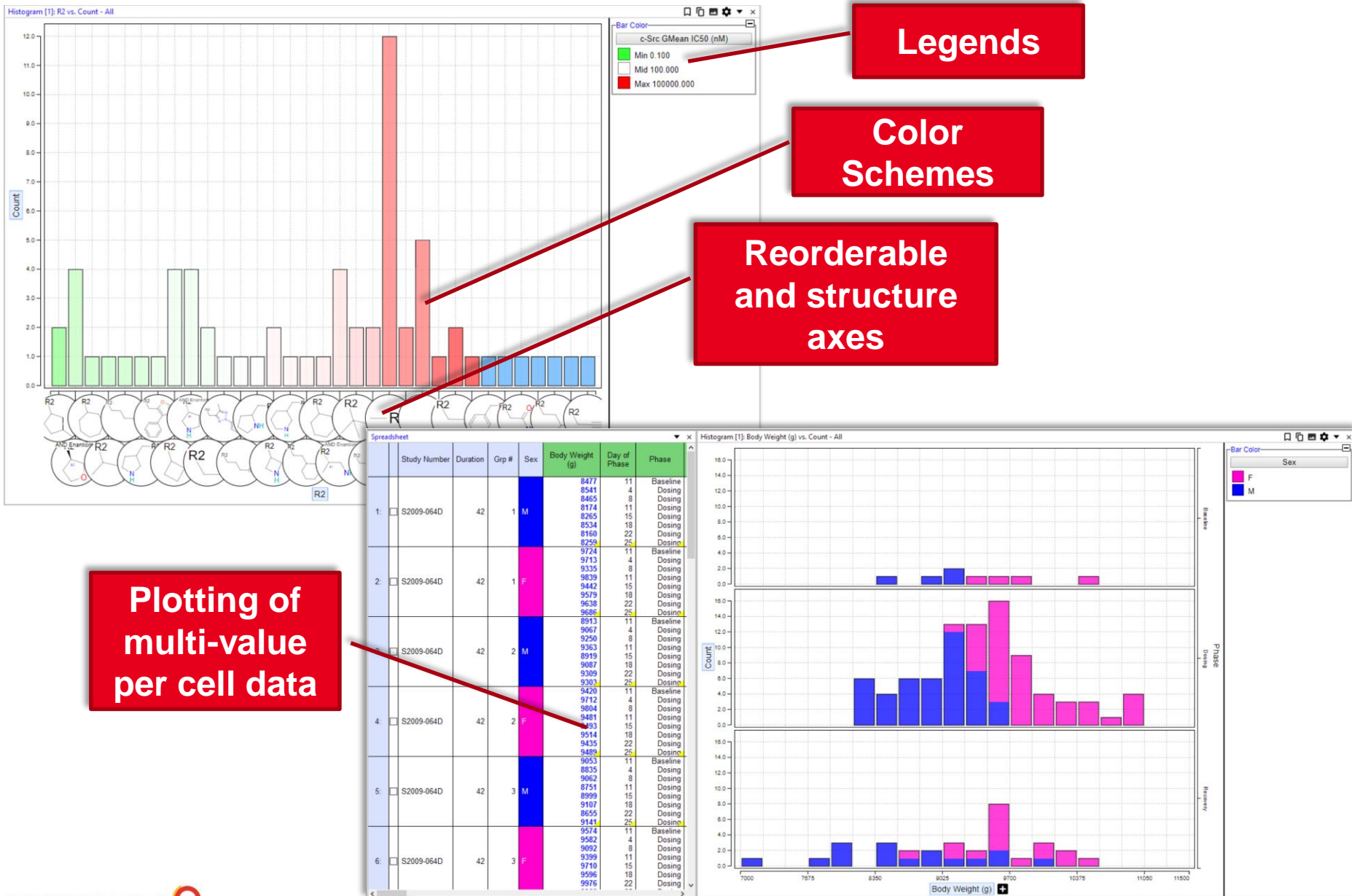
Apply Apply & Close Cancel



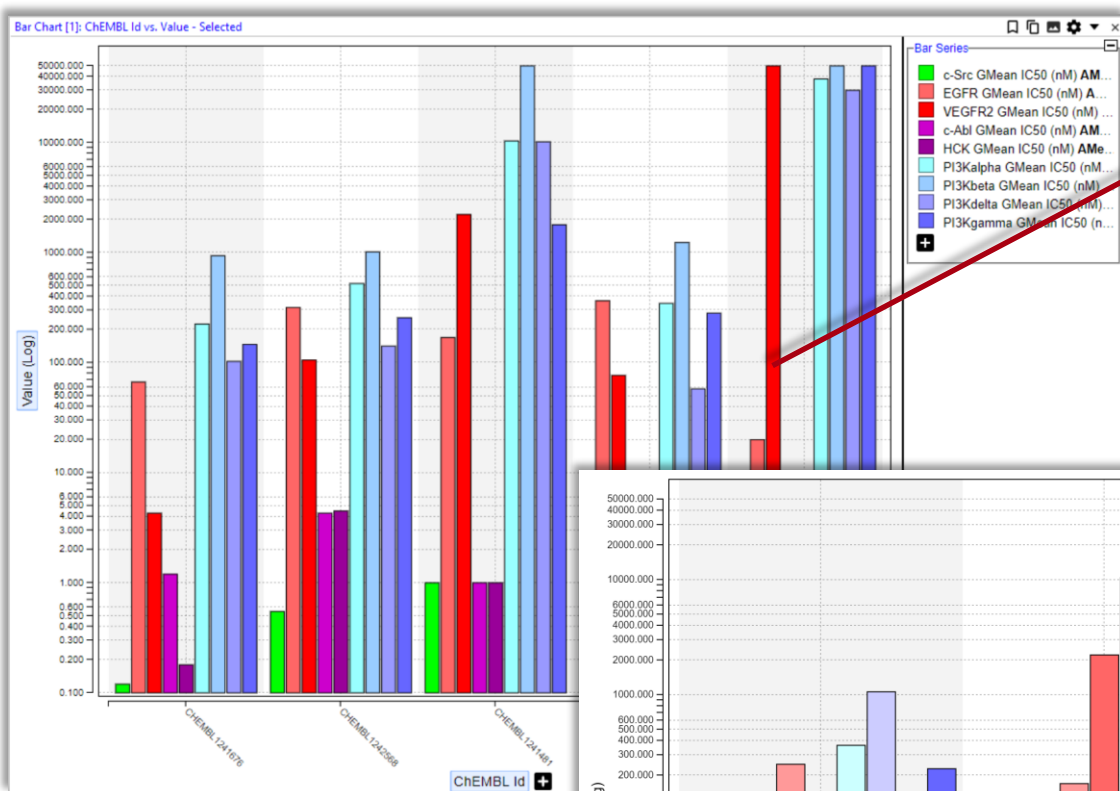
Curve results type in data catalog

spreadsheet cells Rendered from curve parameters

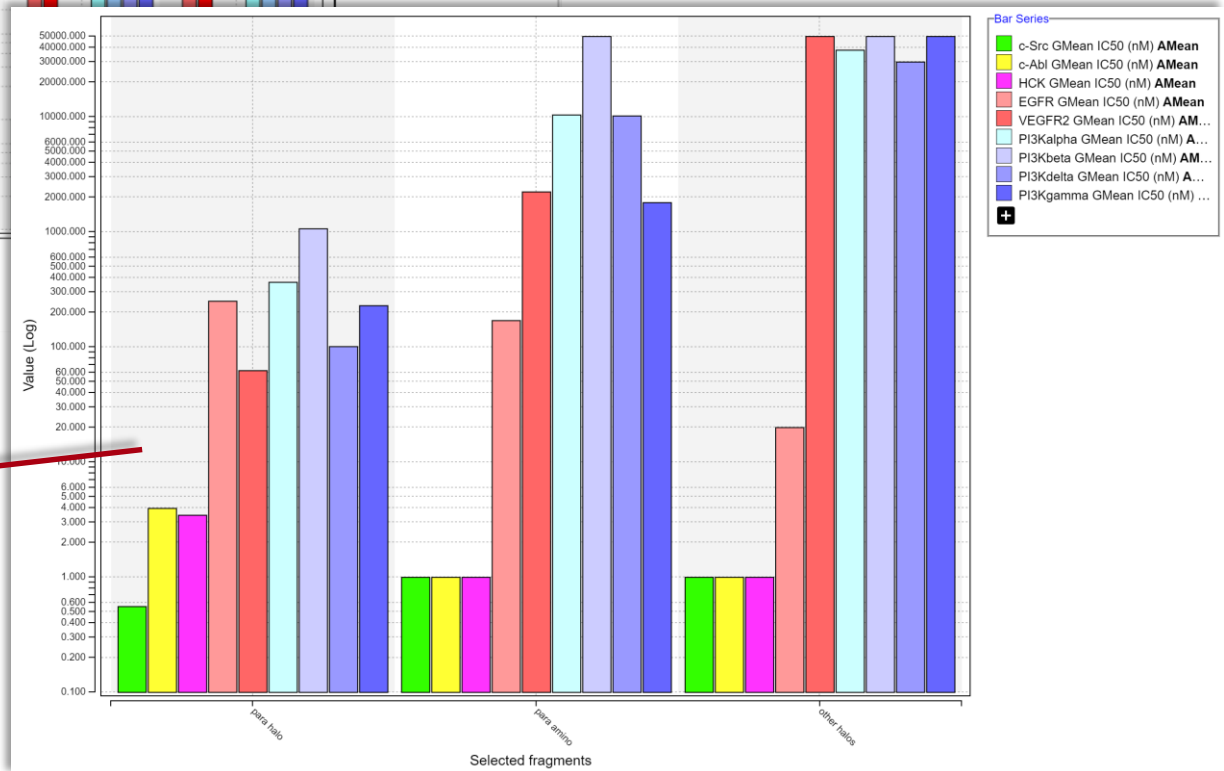
Data Visualization: Updated Histogram (Distribution)



Data Visualization: New Bar Chart (Profiling)

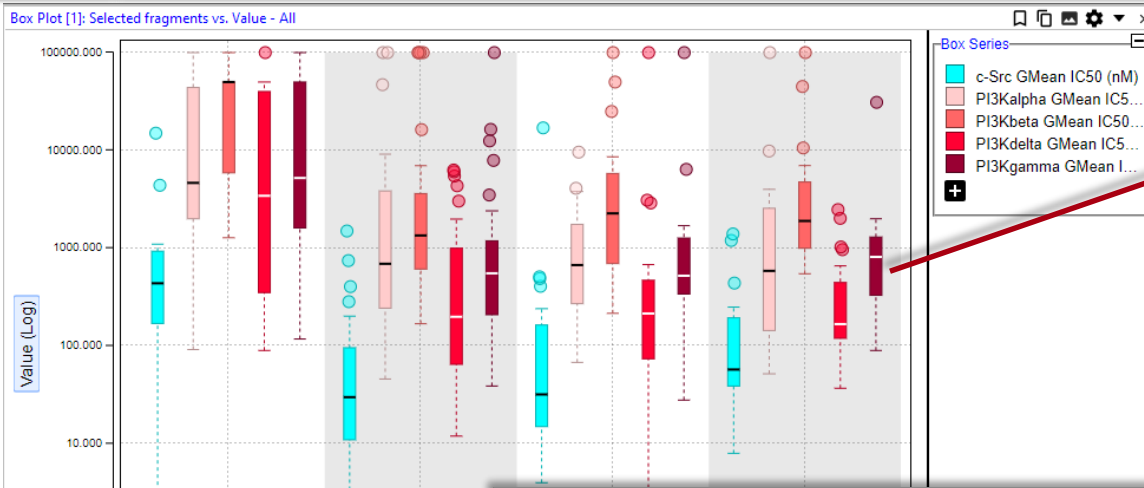


Values for individual molecules over a range of assays

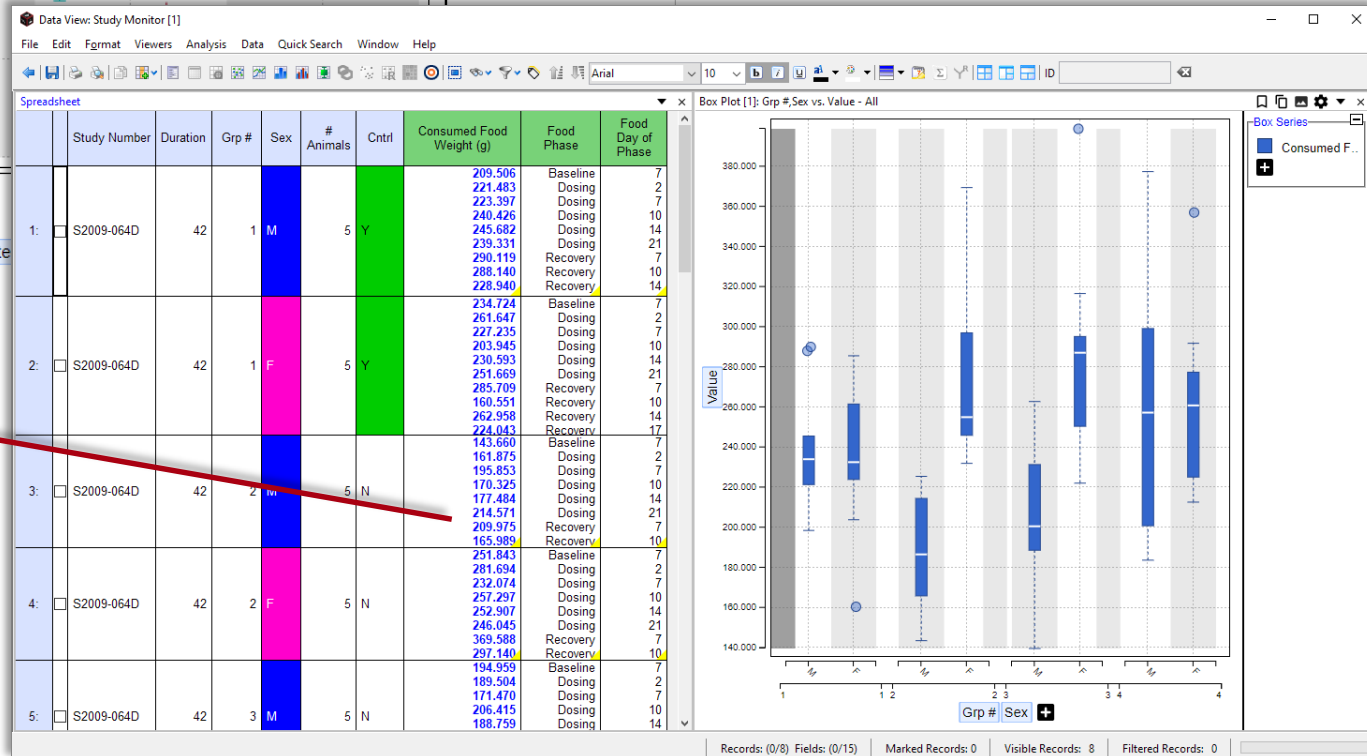


Values for sets of molecules over a range of assays

Data Visualization: New Box Plots (Stats)



Assay result distribution for 5 assays over different molecular series



Plotting of multi-value per cell data

The Devil in the Detail: Handling multi-value per cell

- There is often a choice to make in how to present data...

Pivoted

Compound Number	%Inhibition Concentration: 0.1 uM	%Inhibition Concentration: 1.0 uM	%Inhibition Concentration: 10.0 uM	%Inhibition Concentration: 50.0 uM
Compound A	5	15	60	95

Unpivoted

Compound Number	%Inhibition	Concentration (uM)
Compound A	5	0.1
	15	1.0
	60	10.0
	95	50.0

- A key development goal has been to allow analysis regardless of this choice
 - Data-only constraints, Multi-value per cell equations, In-cell sorting, Multi-value per cell plotting
- Allows far better analysis/interpretation
 - PK data - In vivo data - Panel Assays

Data Visualization: BioProfile Summary

Data Category: Small Molecules

Filter:

- Small Molecules
- Biotherapeutics
- Molecule Synonyms
- Companies
- Journal References
- Targets
- Assays
- Preclinical Studies
- Preclinical Study Groups
- Preclinical Animals
- In-Vitro Results
- Summarized Results
 - Test ID
 - Test Short Name
 - Princ. Result Type
 - Princ. Result Value
 - Condition Names
 - Condition Values

Data Catalog (form)

Configuration to examine data across all assays

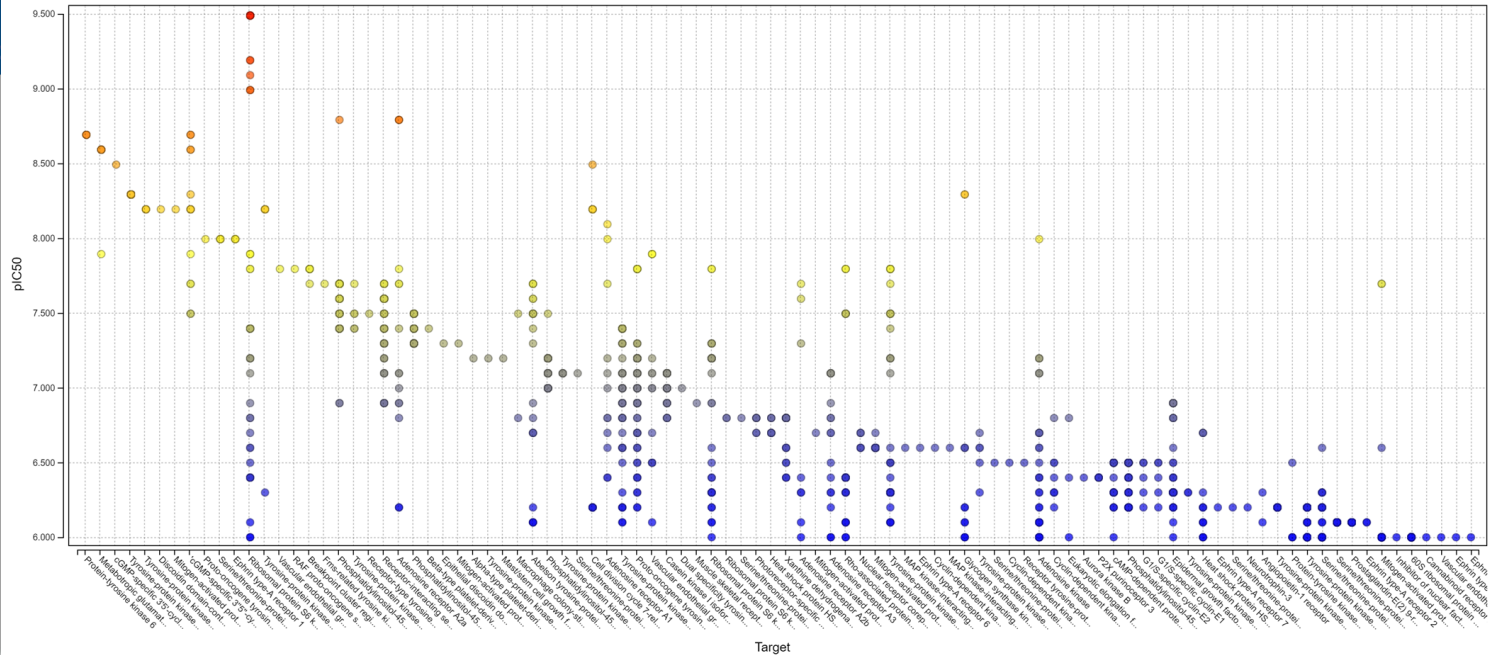
Concatenated Aggregation, Result Type, Unit

Number of used values

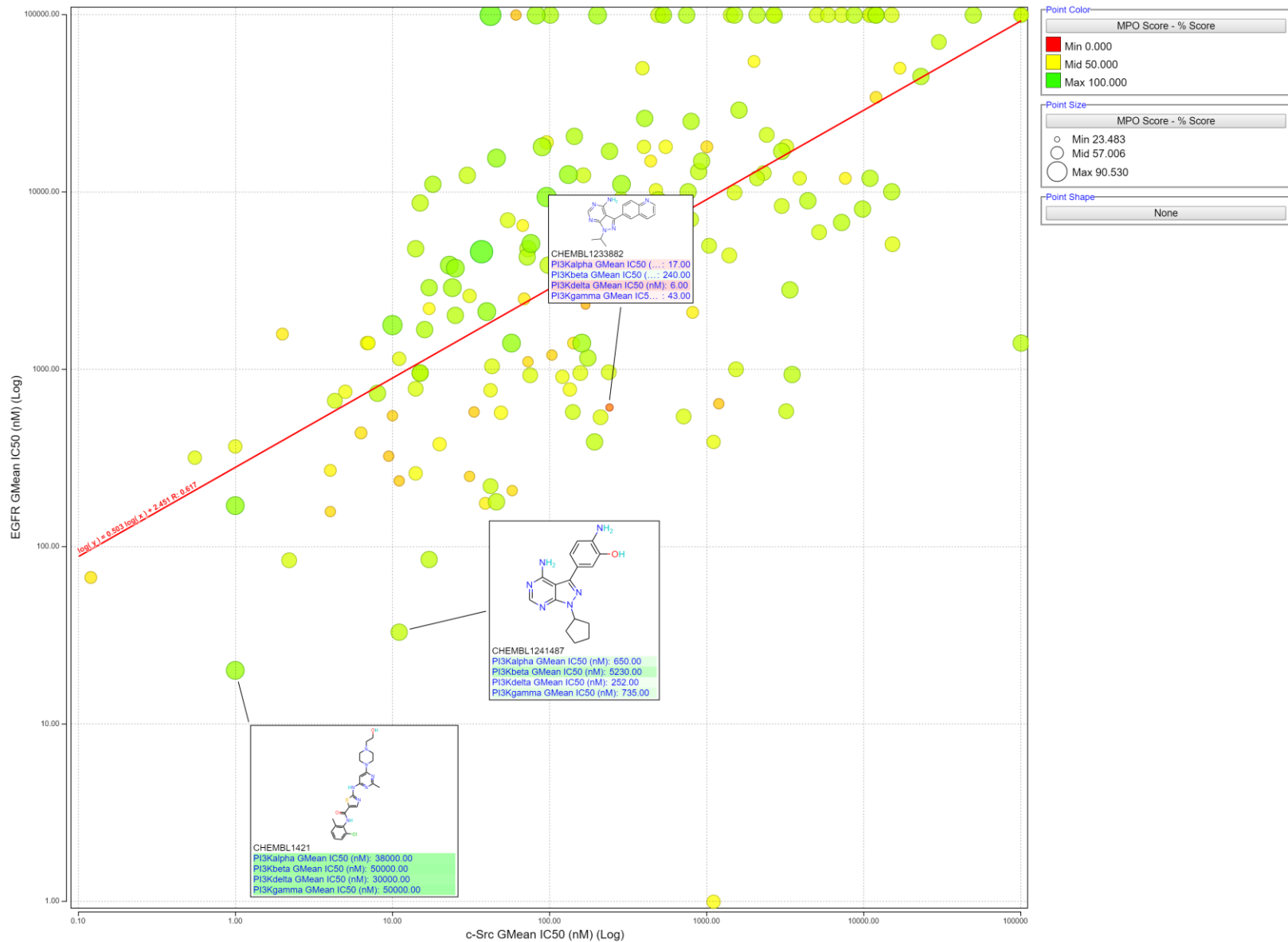
Concatenated Condition Values

Summarized Test ID	Summarized Test Short Name	Summarized Princ. Result Type	Summarized Princ. Result Value	Count Used Princ. Result Value	Summarized Condition Names	Summarized Condition Values	
1	Test1234	c-src kinase	Gmean IC50 (nM)	0.0012	5	Conc (uM):ATP Conc.	10:KM
2	Test1238	HCK kinase	Gmean IC50 (nM)	0.0024	1	Conc (uM):ATP Conc.	10:2
3	Test1349	Rat Plasma	Mean AUC (uM.h)	3.5	1	Admin Route:Gender	IV:Male
4	Test1349	Rat Plasma	Mean Bioavailability (%)	20	1	Admin Route:Gender	IV:Male
5	Test1349	Rat Plasma	Median CL (ml/min/kg)	11.5	1	Admin Route:Gender	IV:Male
6	Test1349	Rat Plasma	Mean t1/2 (h)	1.5	1	Admin Route:Gender	IV:Male
7	Test 2856	HEK proliferation	Gmean IC50 (uM)	0.2	2		

Summarized Results field and the Result

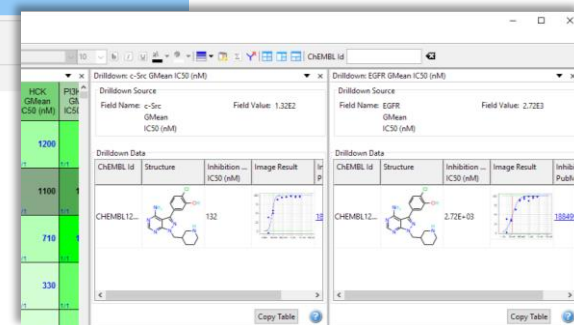
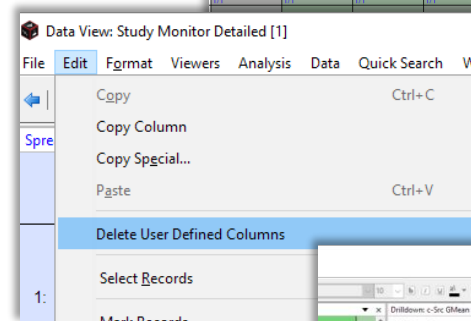
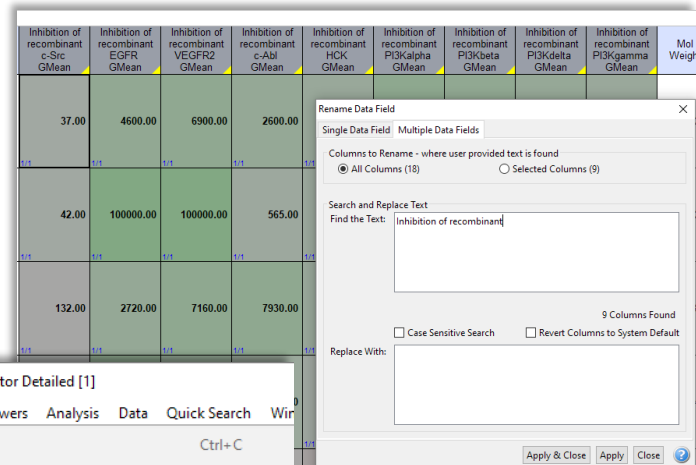


Coming in the next release: Sticky labels



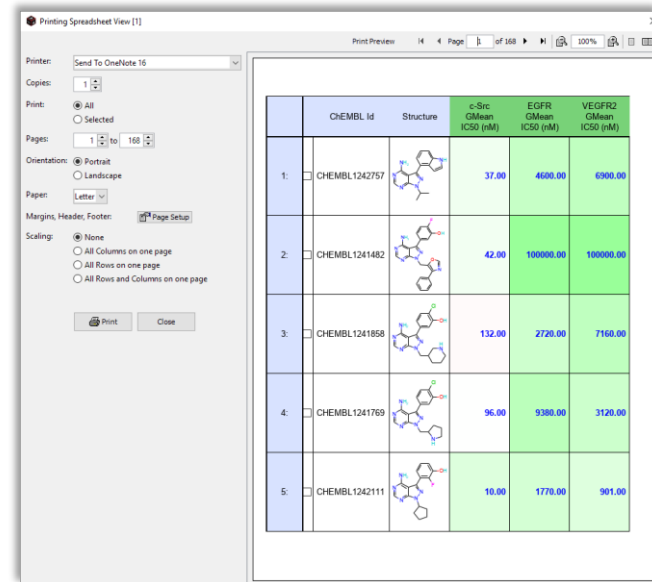
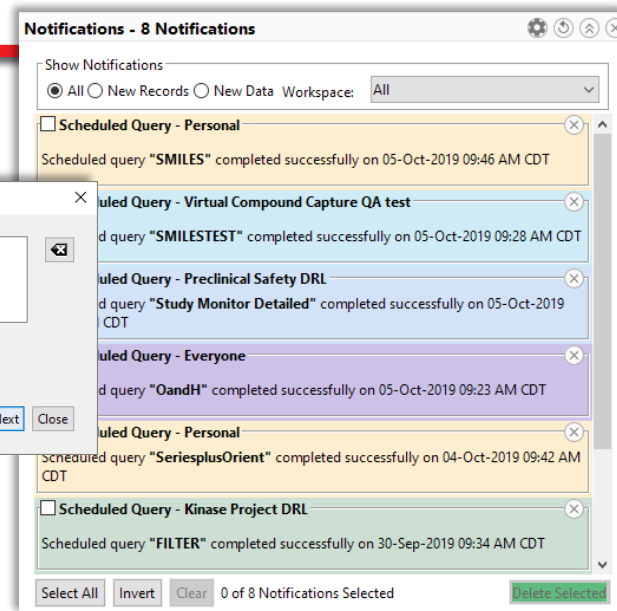
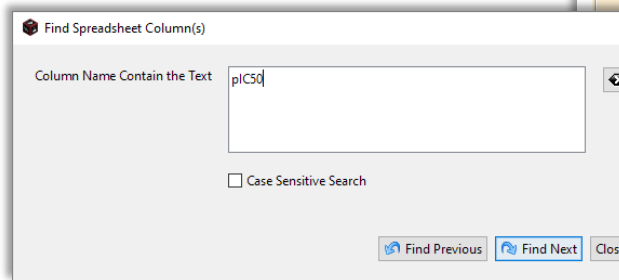
Its also about the little things... 19.1 and 19.6

- Datasets now remember export file type and settings
- Workspace remembers sort order
- Ability to rename multiple columns in one go
- Reduction in size of filter panel/gadgets
- Drag and drop of dataset tabs
- Deletion of user defined columns
 - Including dependent columns
- Query execution – “READY”
- pIC50s – auto-created in the D360 catalog
- Maintaining column order and row height in Drilldown viewer
- ...and many, many more



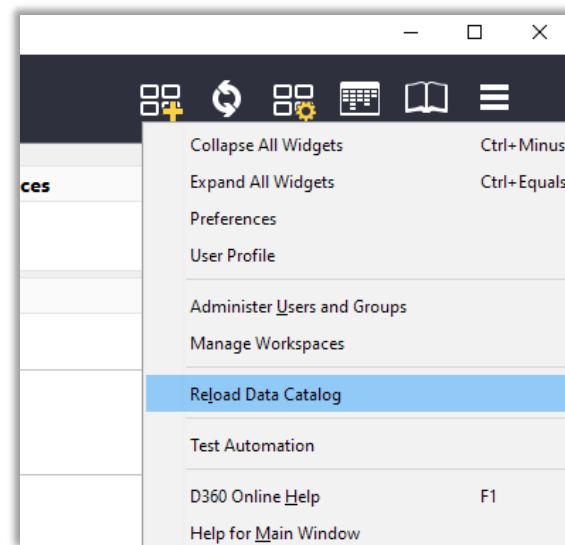
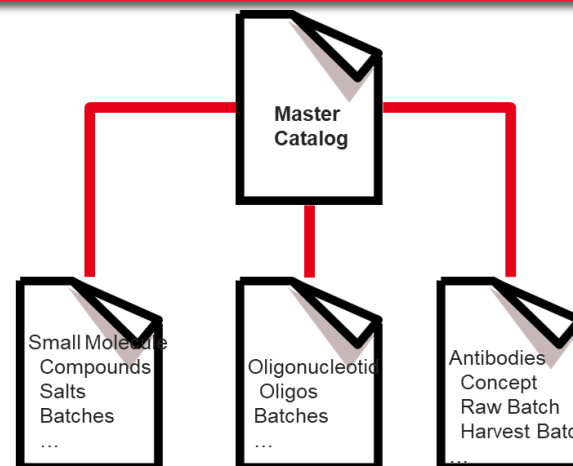
...and this will continue in 20.1

- Updated notifications dashboard widget
- Revamped printing
- Find Column
- Adjustment of font size on chart axes
- Sortable Open/Save dialogs
- Selectively disable Follow-on Queries
- Vastly improved image support
 - Allows High Content Screening workflows
- More in-cell data quality indication
- ...and many, many more



And a little something for administrators

- Data catalog split over multiple files
 - Simplifies data catalog administration vs. everything in one huge file
- Stereo rendering flag config
 - Allows the behavior of enhanced stereochemical flag display to be specified according to specific needs
- Reload catalog from client
 - Simplifies D360 configuration
 - Configuration updates can be observed and tested in the client without the need to restart



**Further Reducing
maintenance overhead**

Later, we'll hear more about the big stuff

- D360 and Biologics
 - After the more important presentations from Roche and Regeneron
- Simplifying deployment
 - The automated test tool and reducing testing overhead
- Interesting workflows
 - Going beyond the normal SAR
- Some popular extensions and configurations of D360
 - What could you be missing in D360's configurable capabilities

Top 3 Exercise

- The Goal:

- To gather feedback on your desired product direction



- Listen, Discuss and Think

- Listen to presenters
- Discuss your needs and desires with others
- Think about what you need over the next year and beyond



- Tomorrow

- We will hand out questionnaire sheets
- Write down your **Top 3 Needs**



- Hand in your sheets tomorrow

- We will collate the feedback and publish after the meeting



Questions?

