

# D360 Test Automation Tool



# D360 Test Automation Tool

## Background:

- Ongoing Certara internal effort around automated testing of D360
- ***UGM attendees requested help with upgrading to new versions, specifically around testing***

## Strategy:

- Provide a mechanism for Certara ***and customers*** to more easily test a new version of D360

## Larger Strategy:

- Provide a extensible admin tool that supports bulk operations on D360 objects

# D360 Test Automation Tool

- **Testing Strategies**
  - The Test Automation Tool supports several types of testing.
  - Start with the simpler testing approaches, and then build up to the more complex testing.
- **Smoke Testing**
  - Ensure that common operations work as expected.
  - Useful for new deploys and configuration changes.
  - Any errors are logged for later review.
- **Functional Testing**
  - More complete testing, but tool eliminates the need for any manual operations, other than visual inspection of results.
  - Screenshots of the resulting datasets, can be easily reviewed.
  - The complete dataset files can be opened and reviewed if needed.
- **Regression Testing**
  - Detailed comparison of results against expected (or “master”) results, either from another D360 server, or from an earlier run of the Test Automation Tool.
  - Differences are logged by the tool.
  - Requires precise queries and stable data in order to avoid false failures.

# D360 Test Automation Tool

Query List Filter

Query List Operators

Query List

The screenshot shows the D360 Admin Automation Tool interface. At the top, there are buttons for 'Load List...', 'Save List...', 'Add to List...', 'Delete Selected from List', and 'Clear List'. Below this is a table of 'D360 Objects' with columns for Name, Type, and Path. The table contains several entries, including 'Bar Chart - Hist Filter SN', 'Bar Chart - Lines and Trellis - Multiple X-axis data fields', 'Compounds in screening queue or submitted', 'Discovery: HIV with Viewers', and 'Drugs by Company'. Below the table, there are 'Action Controls' including a dropdown menu for 'Perform Action on Selected Objects' (set to 'Execute Queries in D360 Client and Compare Results'), 'Run', and 'Cancel' buttons. Underneath are 'Action Details' for 'Export Results', 'Export Location', and 'Master Results'. There are also checkboxes for 'Preserve Results History' and 'Standardize Results'. At the bottom, there is a 'Results' table with columns for Name, Status, and Details. The table shows the status of each query, with 'in cell sort' highlighted in green and 'Drugs by Company' in red. A status bar at the bottom right indicates 'Running: 6 of 8'.

Name	Type	Path
Bar Chart - Hist Filter SN	Query Tem...	\\WS.Personal.scott\Test Automation\Bar Chart - Hist Filter SN
Bar Chart - Lines and Trellis - Multiple X-axis data fields	Query Tem...	\\WS.Personal.scott\Test Automation\Bar Chart - Lines and T...
Compounds in screening queue or submitted	Query Tem...	\\WS.Personal.scott\Test Automation\Compounds in screeni...
Discovery: HIV with Viewers	Query Tem...	\\WS.Personal.scott\Test Automation\Discovery: HIV with Vie...
Drugs by Company	Query Tem...	\\WS.Personal.scott\Test Automation\Drugs by Company

#Objects: 8 #Invalid: 0 #Filtered: 0

Perform Action on Selected Objects: Execute Queries in D360 Client and Compare Results Run Cancel

Action Details

Export Results: Template,QQuery,Shift-Copy,SQL,D360 Dataset File (d360d),Excel,Comma-Separated Text (CSV),Screen Capture,Viewe...

Export Location: C:\Temp\TestAutomation\demost196\KBList

Master Results: C:\Temp\TestAutomation\demost196\KBList\Master

Preserve Results History  Standardize Results

Results Analyze

Name	Status	Details
Bar Chart - Lines and Trellis - Multiple X-axis data fields	Success	Successful run
Compounds in screening queue or submitted	Success	Successful run
Discovery: HIV with Viewers	Success	Successful run
Drugs by Company	Failure	Differences in exported items: ViewerImages
in cell sort	Running	Exporting Excel PROCESS_STRUCTURES 62%

Running: 6 of 8

Action Selector

Action Controls

Action Details

Standardize Results

Eliminate unimportant differences (e.g. data order)

Preserve Results History

Track result history by date and time

Analyze Result History

View results of multiple runs over time

Action Results

Results of the Action on each query in the list

# Use Case 1 – Smoke Testing the D360 Server

- In the simplest scenario, want to run hundreds of queries (with minimal effort) and verify no anomalies.
- Only current “automated” option is Scheduled Queries
  - Works, but not optimal
  - Can be inconvenient to set up for 10’s/100’s of queries
  - May require server restarts to restart the SQ’s
  - Might interfere with users SQ’s
- DEMO

# Use Case 1 – Smoke Testing the D360 Server

The screenshot displays the D360 Admin Automation Tool interface. At the top, the window title is "D360 Admin Automation Tool". Below the title bar, there is a search field for "D360 Objects" and several buttons: "Load List...", "Save List...", "Add to List...", "Delete Selected from List", and "Clear List".

The main area contains a table with the following columns: "Name", "Type", and "Path". The table lists several objects, including "Bar Chart - Lines and Trellis - Multiple X-axis data fields", "Compounds in screening queue or submitted", "Discovery: HIV with Viewers", "Drugs by Company", "in cell sort", and "Kinase Project SF".

Below the table, there are statistics: "#Objects: 7 #Invalid: 0 #Filtered: 0".

The "Perform Action on Selected Objects:" dropdown is set to "Execute Queries on D360 Server", with "Run" and "Cancel" buttons.

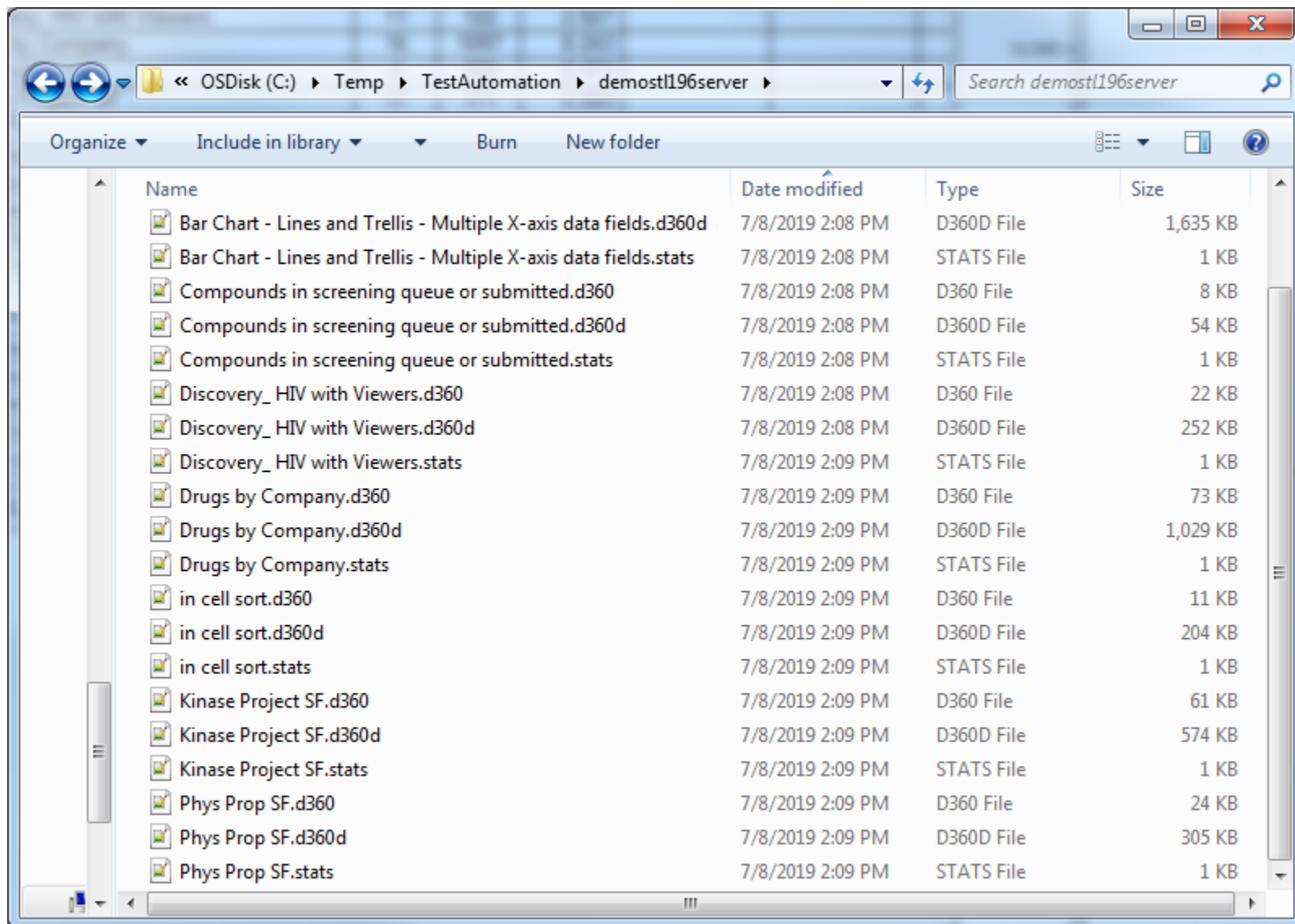
The "Action Details" section includes:

- Export Results: Template, D360 Dataset File (d360d) (with a "Manage Servers..." button)
- D360 Server: 1: d360demostl:8380 - 19.6.2
- Export Location: C:\Temp\TestAutomation\demostl196server
- Preserve Results History

The "Results" section shows a table with columns: "Name", "Status", and "Details". The table lists the same objects as above, with their execution status and details. A context menu is open over the "Discovery: HIV with Viewers" row, showing options: "Generate List from Failed Tests", "View Template", and "View D360 Dataset File (d360d)".

At the bottom right of the results table, the word "Complete" is displayed.

# Use Case 1 – Smoke Testing the D360 Server



Name	Date modified	Type	Size
Bar Chart - Lines and Trellis - Multiple X-axis data fields.d360d	7/8/2019 2:08 PM	D360D File	1,635 KB
Bar Chart - Lines and Trellis - Multiple X-axis data fields.stats	7/8/2019 2:08 PM	STATS File	1 KB
Compounds in screening queue or submitted.d360	7/8/2019 2:08 PM	D360 File	8 KB
Compounds in screening queue or submitted.d360d	7/8/2019 2:08 PM	D360D File	54 KB
Compounds in screening queue or submitted.stats	7/8/2019 2:08 PM	STATS File	1 KB
Discovery_HIV with Viewers.d360	7/8/2019 2:08 PM	D360 File	22 KB
Discovery_HIV with Viewers.d360d	7/8/2019 2:08 PM	D360D File	252 KB
Discovery_HIV with Viewers.stats	7/8/2019 2:09 PM	STATS File	1 KB
Drugs by Company.d360	7/8/2019 2:09 PM	D360 File	73 KB
Drugs by Company.d360d	7/8/2019 2:09 PM	D360D File	1,029 KB
Drugs by Company.stats	7/8/2019 2:09 PM	STATS File	1 KB
in cell sort.d360	7/8/2019 2:09 PM	D360 File	11 KB
in cell sort.d360d	7/8/2019 2:09 PM	D360D File	204 KB
in cell sort.stats	7/8/2019 2:09 PM	STATS File	1 KB
Kinase Project SF.d360	7/8/2019 2:09 PM	D360 File	61 KB
Kinase Project SF.d360d	7/8/2019 2:09 PM	D360D File	574 KB
Kinase Project SF.stats	7/8/2019 2:09 PM	STATS File	1 KB
Phys Prop SF.d360	7/8/2019 2:09 PM	D360 File	24 KB
Phys Prop SF.d360d	7/8/2019 2:09 PM	D360D File	305 KB
Phys Prop SF.stats	7/8/2019 2:09 PM	STATS File	1 KB

# Use Case 1 – Smoke Testing the D360 Server

- DEMO
- ***With 19.6 Test Automation Tool***
  - *Can easily run an arbitrary list of queries on the server, unattended, anytime of day, without interfering with users SQs.*



# Use Case 2 – Functional Testing of the D360 Client

- Only option currently is running the D360 client and repeatedly opening and running N queries
  - Requires a person
  - Manual, and can be tedious
  - Can be time consuming (depending on query speed)
- DEMO

# Use Case 2 – Exporting Results

- **The Test Automation Tool supports exporting various files types as part of query execution:**
  - Microsoft Excel
  - Comma Separated Values (CSV)
  - Spotfire CSV – Comma delimited file, suitable for easy import into Spotfire
  - Tab Separate Values (TSV)
  - D360 Template – Original D360 query
  - D360 Dataset – Full D360 Dataset, including data and visualizations
  - Screen Capture – Full screenshot of the complete D360 query and macro results
  - Viewer Images - Screenshot of each individual D360 view
  - Template – D360 spreadsheet or form query template
  - SQL - SQL based on QQuery and Shift-Copy details
  - QQuery - D360 internal basic query definition
  - Shift-Copy – D360 internal metadata for query columns
- **Preserve Results History**
- The “Preserve Results History” option will force the creation of a separate output folder for each execution, with a folder name including the D360 version plus date and time.
- **Standardize Results**
- D360 datasets will sometimes display data in different (row order from run to run. This is as expected and is due to the fact the underlying relational database(s) do not return data in a defined order, but can be misleading when reviewing results. Using the “Standardize Results” option, the Test Automation tool will automatically sort the resulting data set. The data will be sorted by the category key for the query in ascending order.

# Use Case 2 – Functional Testing of the D360 Client

D360 Admin Automation Tool

D360 Objects

Name	Type	Path
Bar Chart - Lines and Trellis - Multiple X-axis data fields	Query Tem...	\\WS.Personal.scott\Test Automation\Bar Chart - Lines and T...
Compounds in screening queue or submitted	Query Tem...	\\WS.Personal.scott\Test Automation\Compounds in screeni...
Discovery: HIV with Viewers	Query Tem...	\\WS.Personal.scott\Test Automation\Discovery: HIV with Vie...
Drugs by Company	Query Tem...	\\WS.Personal.scott\Test Automation\Drugs by Company
in cell sort	Query Tem...	\\WS.Personal.scott\Test Automation\in cell sort
Kinase Project SE	Query Tem...	\\WS.Personal.scott\Test Automation\Kinase Project SE

#Objects: 7 #Invalid: 0 #Filtered: 0

Perform Action on Selected Objects:

Action Details

Export Results:

Export Location:

Preserve Results History

Results

Name	Status	Details
Bar Chart - Lines and Trellis - Multiple X-axis data fields	Success	Successful run
Compounds in screening queue or submitted	Success	Successful run
Discovery: HIV with Viewers	Success	Successful run
Drugs by Company	Running	Exporting Excel PROCESS_STRUCTURES 83%

Running: 4 of 7

# Use Case 2 – Functional Testing of the D360 Client

The screenshot displays a Windows file explorer window with the following path: S:\18RDWD-HWR0BP1 \> OSDisk (C:) \> Temp \> TestAutomation \> demost196client \> 19.6.2 - 2019.07.10.17.39.02. The file list includes:

- in cell sort.xlsx (Microsoft Excel W...)
- in cell sort\_viewer\_Spreadsheet[SPREADSHEET.1].png (PNG image)
- Phys Prop SF.csv (Microsoft Excel C...)
- Phys Prop SF.d360 (D360 File)
- Phys Prop SF.d360d (D360D File)
- Phys Prop SF.png (PNG image)
- Phys Prop SF.stats (STATS File)
- Phys Prop SF.xlsx (Microsoft Excel W...)
- Phys Prop SF\_viewer\_Histogram[JFX\_HISTOGRAM.3]... (PNG image)
- Phys Prop SF\_viewer\_Scatter Plot[JFX\_SCATTERPLOT.... (PNG image)
- Phys Prop SF\_viewer\_Spreadsheet[SPREADSHEET.1].p... (PNG image)
- Phys Prop SF\_viewer\_Structure All[SARMAP.2].png (PNG image)
- Simple 1.csv (Microsoft Excel C...)
- Simple 1.d360 (D360 File)
- Simple 1.d360d (D360D File)
- Simple 1.png (PNG image)
- Simple 1.stats (STATS File)
- Simple 1.xlsx (Microsoft Excel W...)
- Simple 1\_viewer\_Scatter Plot[JFX\_SCATTERPLOT.2].png (PNG image)
- Simple 1\_viewer\_Spreadsheet[SPREADSHEET.1].png (PNG image)

On the right, a preview window shows a table with columns: CHEMBL ID, STATUS, Mol Weight (g/mol), and LogP (cLogP). The data is as follows:

CHEMBL ID	STATUS	Mol Weight (g/mol)	LogP (cLogP)
1		344.393	2.839
2		383.403	2.113
3		162.200	1.269
4		361.170	-1.370
5		309.343	1.163

Below the table is a scatter plot with 'Mol Weight (g/mol)' on the x-axis and 'LogP (cLogP)' on the y-axis. The plot shows five data points corresponding to the rows in the table above. The plot area includes a legend for 'Font Color', 'Font Size', and 'Font Shape', each with a 'None' option.

# Use Case 2 – Functional Testing of the D360 Client

- DEMO
- *With 19.6 Test Automation*
  - *Can easily run an arbitrary list of queries **in the client**, unattended, anytime of day, and **quickly review the results later, including visualizations.***

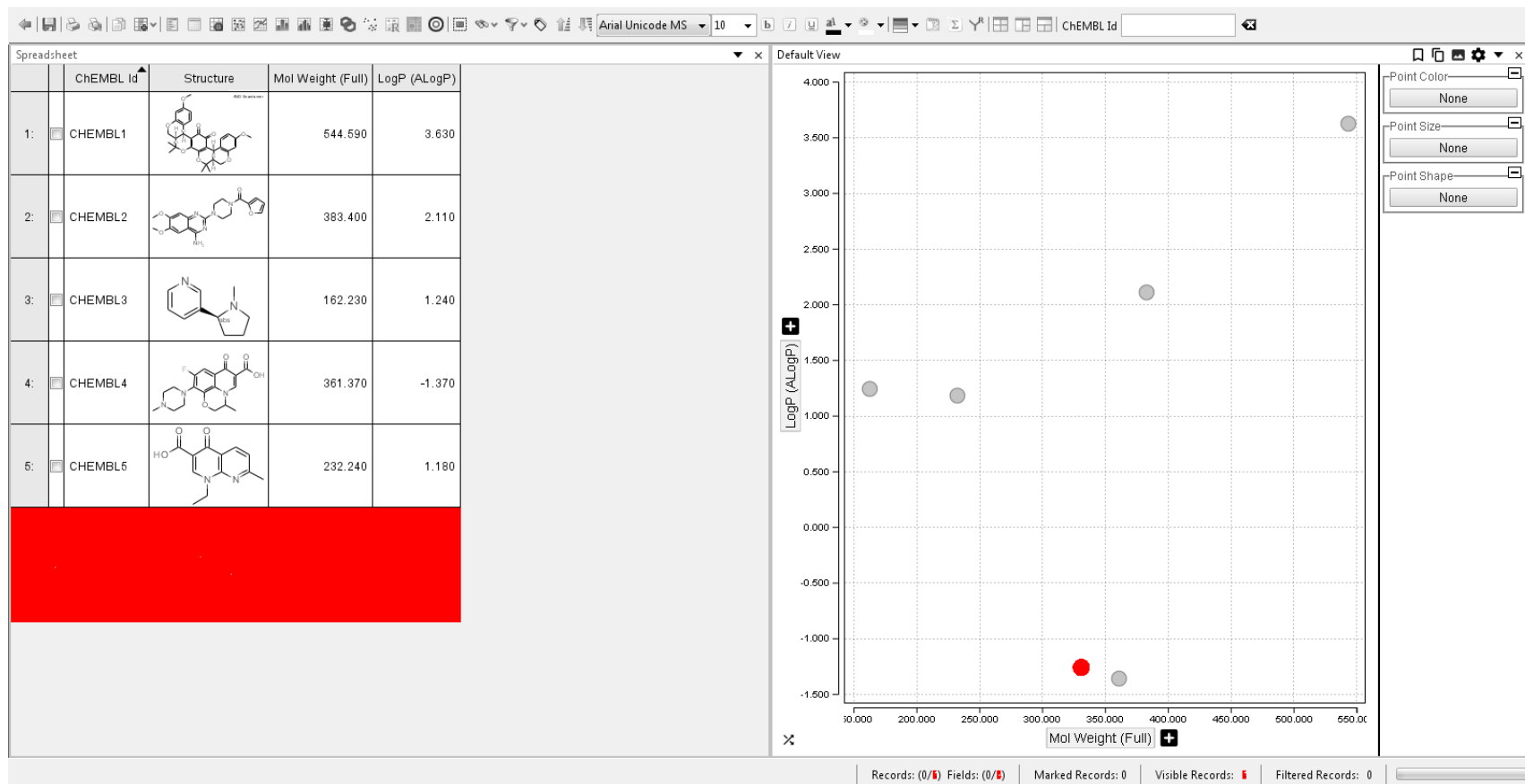
# Use Case 3 – Regression Testing

- Confirm that results are as exactly as expected.
  - Usually involves comparing results from the new D360 version against results from the current D360 production deploy
- Only option currently is for a human to manually look at the output from the old and new versions.
- DEMO

# Use Case 3 – CSV Compare

Line #0	ChEMBL Id	Structure	Mol Weight (Full)	LogP (ALogP)	Marked
Line #6	CHEMBL8	<chem>Fc1c(cc2c(c1)C(=O)C(=CN2C3CC3)C(=O)O)N4CCNCC4</chem>	331.340	-1.270	UNMARKED

# Use Case 3 – Screenshot Compare





# Use Case 3 – Excel Spreadsheet Compare

Spreadsheet Compare - File 1: [Dataset2.xlsx] - File 2: [Dataset1.xlsx]

Home  
Compare Files Show Details Show Formulas View Export Results Copy Results to Clipboard Information Options Help

	A	B	C	D		A	B	C	D	E	
1	CHEMBL Id	Structure	Canonical SMILES	Mol Weight (Free Base)		1	CHEMBL Id	Structure	Canonical S	Mol Weight (Free Base)	Mol Weight (Full)
2	CHEMBL70		[O-][S+](Cc1ccc	353.520		2	CHEMBL70		[O-][S+](C	353.520	353.520
3	CHEMBL70		CNc1ccc(n1)N1	349.430		3	CHEMBL70		CCNc1cccc	349.430	349.430
4	CHEMBL70		CC(CCc1cccc1)N	365.510		4	CHEMBL70		CC(CCc1cc	365.470	365.470
5	CHEMBL70		Nc1nc(O)c2c(n1	365.220		5	CHEMBL70		Nc1nc(O)c	365.220	365.220
6	CHEMBL70		CCC(Oc(=O)c1nc	361.820		6	CHEMBL70		CCC(Oc(=	361.820	361.900
7	CHEMBL70		Cc1cccc(c1)N1C	231.300		7	CHEMBL70		Cc1cccc(c1	231.300	231.300
8	CHEMBL70		CNc1ncnc2c1nc2	257.270		8	CHEMBL70		CNc1ncnc2	257.270	257.270
9	CHEMBL70		CNc1ncnc2c1nc2	284.270		9	CHEMBL70		CNc1ncnc2	284.270	284.270
10	CHEMBL70		SC(=Nc1ccc(cc1C	415.570		10	CHEMBL70		SC(=Nc1cc	415.570	415.570
11	CHEMBL70		SC(=Nc1ccc(cc1C	401.550		11	CHEMBL70		SC(=Nc1cc	401.550	401.550

D360 Export

Enable	Option	Sheet	Cell	Value 1	Value 2	Change Description
<input type="checkbox"/>	Select All	D360 Export				Added Column E.
<input checked="" type="checkbox"/>	Entered Values	D360 Export				Added Row 17.
<input checked="" type="checkbox"/>	Calculated Values	D360 Export				Added Row 19.
<input checked="" type="checkbox"/>	Formulas	D360 Export	A17		CHEMBL7084	Entered Value Added.
<input checked="" type="checkbox"/>	SysGen Formulas	D360 Export	A19		CHEMBL7087	Entered Value Added.
<input type="checkbox"/>	SysGen Formulas Error	D360 Export	C17		O=c1[nH]c(=O)...	Entered Value Added.
<input type="checkbox"/>	Structural	D360 Export	C19		NCCc1ccc(cc1...	Entered Value Added.
<input checked="" type="checkbox"/>	Names	D360 Export	D4	365.510 (365.51)	365.470 (365.47)	Entered Value Changed.
<input checked="" type="checkbox"/>	SysGen Names	D360 Export	D17		474.350 (474.35)	Entered Value Added.
<input type="checkbox"/>	SysGen Names Error	D360 Export	D19		200.260 (200.26)	Entered Value Added.
<input checked="" type="checkbox"/>	Macros	D360 Export	E1		Mol Weight (Full)	Entered Value Added.
<input type="checkbox"/>	...	D360 Export	E2		353.520 (353.52)	Entered Value Added.
<input type="checkbox"/>	...	D360 Export	E3		349.430 (349.43)	Entered Value Added.
<input type="checkbox"/>	...	D360 Export	E4		365.470 (365.47)	Entered Value Added.
<input type="checkbox"/>	...	D360 Export	E5		365.220 (365.22)	Entered Value Added.
<input type="checkbox"/>	...	D360 Export	E6		361.900 (361.9)	Entered Value Added.

Ready - File 1: [Dataset2.xlsx] - File 2: [Dataset1.xlsx] - Total Displayed Items: 30

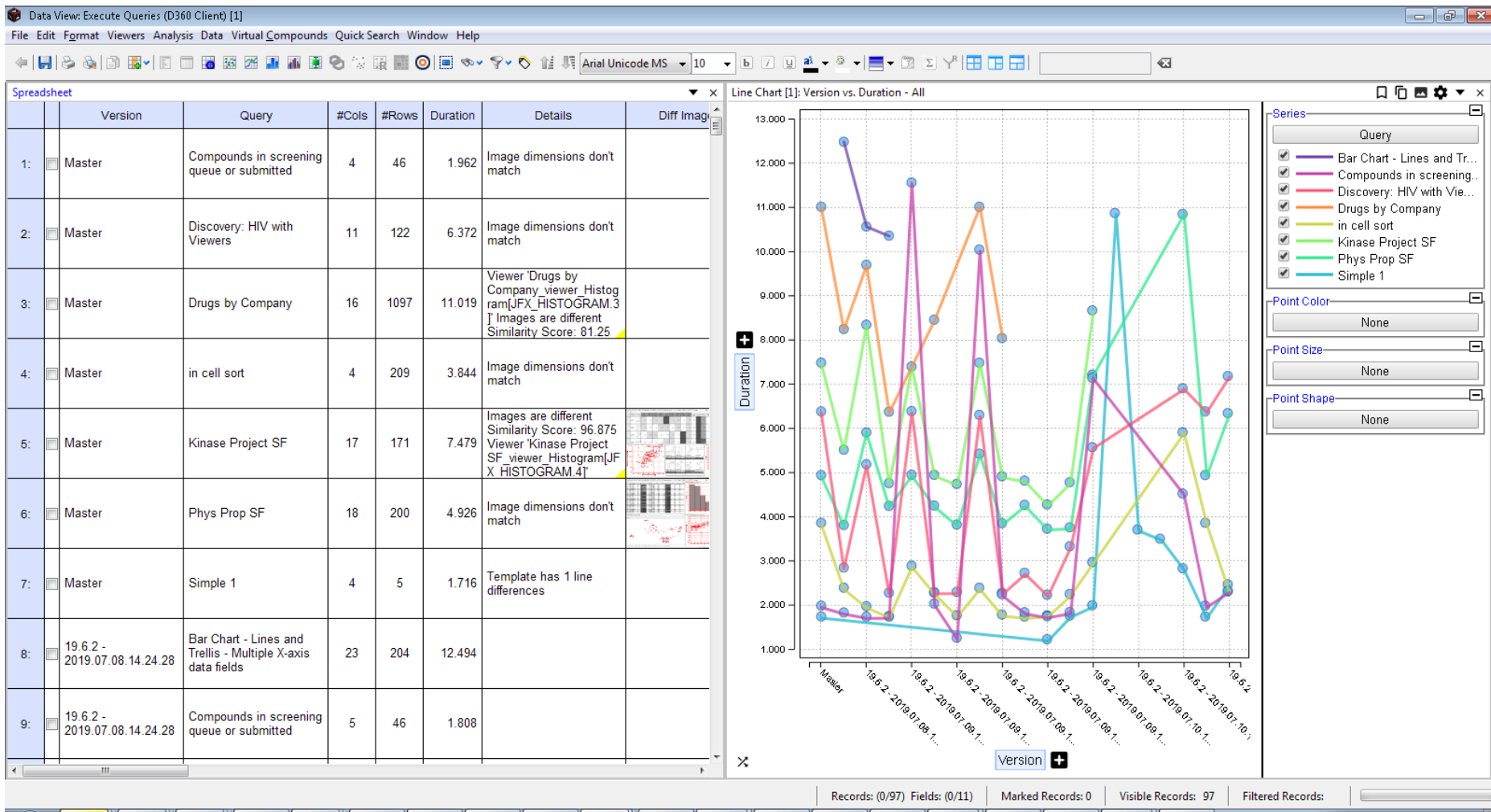
# Use Case 3 – Regression Testing

- DEMO
- *With 19.6 Test Automation*
  - *Can easily run an arbitrary list of queries in the client, unattended, anytime of day, and quickly review the results later, including visualizations, **and automatically compare the results against an expected set of results.***

# Use Case 4 – Performance/Trends

- “Is query performance stable over time?”
- “I added an index to a database table. Did it help?”
- DEMO
- *With 19.6 Test Automation*
  - *Can easily run an arbitrary list of queries in the client, unattended, anytime of day, and quickly review the results later, including visualizations, and automatically compare the results against an expected set of results, **and analyze results over time.***

# Use Case 4 – Performance/Trends



# Other Operations

- ***Export Queries***
  - Allows easily exporting many queries to the filesystem in a single operation.
  - Can be useful as a way to “snapshot” queries and/or to access the queries from another D360 environment.
- ***Execute Queries on D360 Servers and Compare Results***
  - Execute against one server, and then immediately execute against a different server.
  - Minimizes differences to changing data.
  - Will be most useful for D360 19.6+ versions.

Questions?

