1001 Configurations

A potpourri of popular extensions, add-ons and configurable options in D360

Dr. Fabian Rauscher | D360 UGM 2019

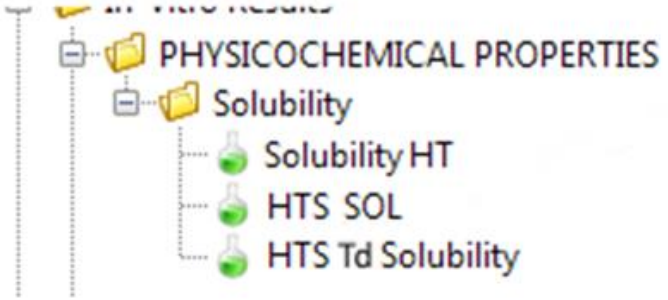
Preface

- D360 flexible configurable system
  - Core product installer for all customers
  - Customer specific configuration & plugins
- Data catalog mapping customer data sources into D360
- Extendable through configuration, scripting, coding

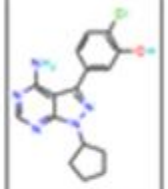
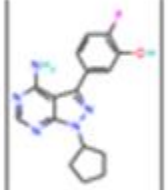
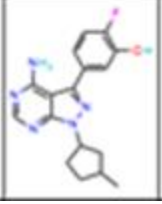
A … like Assays

The Evergreens: Super Assays & Assays Groups

- Results from multiple, equivalent assays represented in more columns than necessary.



Spreadsheet View [1]

		ChEMBL Id	Structure	Solubility HT Mean SOL (ug/ml) pH: 4.500	Solubility HT Mean SOL (ug/ml) pH: 6.800	HTS SOL Mean Solubility (ug/ml) pH: 4.500	HTS SOL Mean Solubility (ug/ml) pH: 7.400	HTS Td Solubility Mean Sol (ug/ml) pH: 4.500	HTS Td Sol Mean Sol (ug/ml) pH: 6.8
1:		CHEMBL1241676		0.130	0.110				
2:		CHEMBL1242568				0.650	2.050		
3:		CHEMBL1242656						320.000	22

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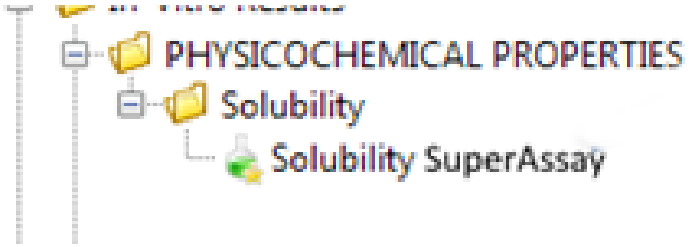
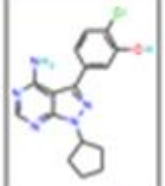
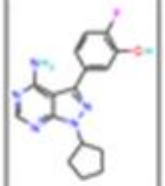
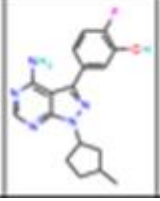
The Evergreens: Super Assays & Assays Groups

- Same assays combined into a Super Assay so they appear as single assay



Spreadsheet View [1]

		ChEMBL Id	Structure	Solubility SuperAssay Mean Solubility (ug/ml) pH: 4.500	Solubility SuperAssay Mean Solubility (ug/ml) pH: 6.800	Solubility SuperAssay Mean Solubility (ug/ml) pH: 7.400
1:		CHEMBL1241676		0.130	0.110	
2:		CHEMBL1242568		0.650		2.050
3:		CHEMBL1242656		320.000	2200.000	

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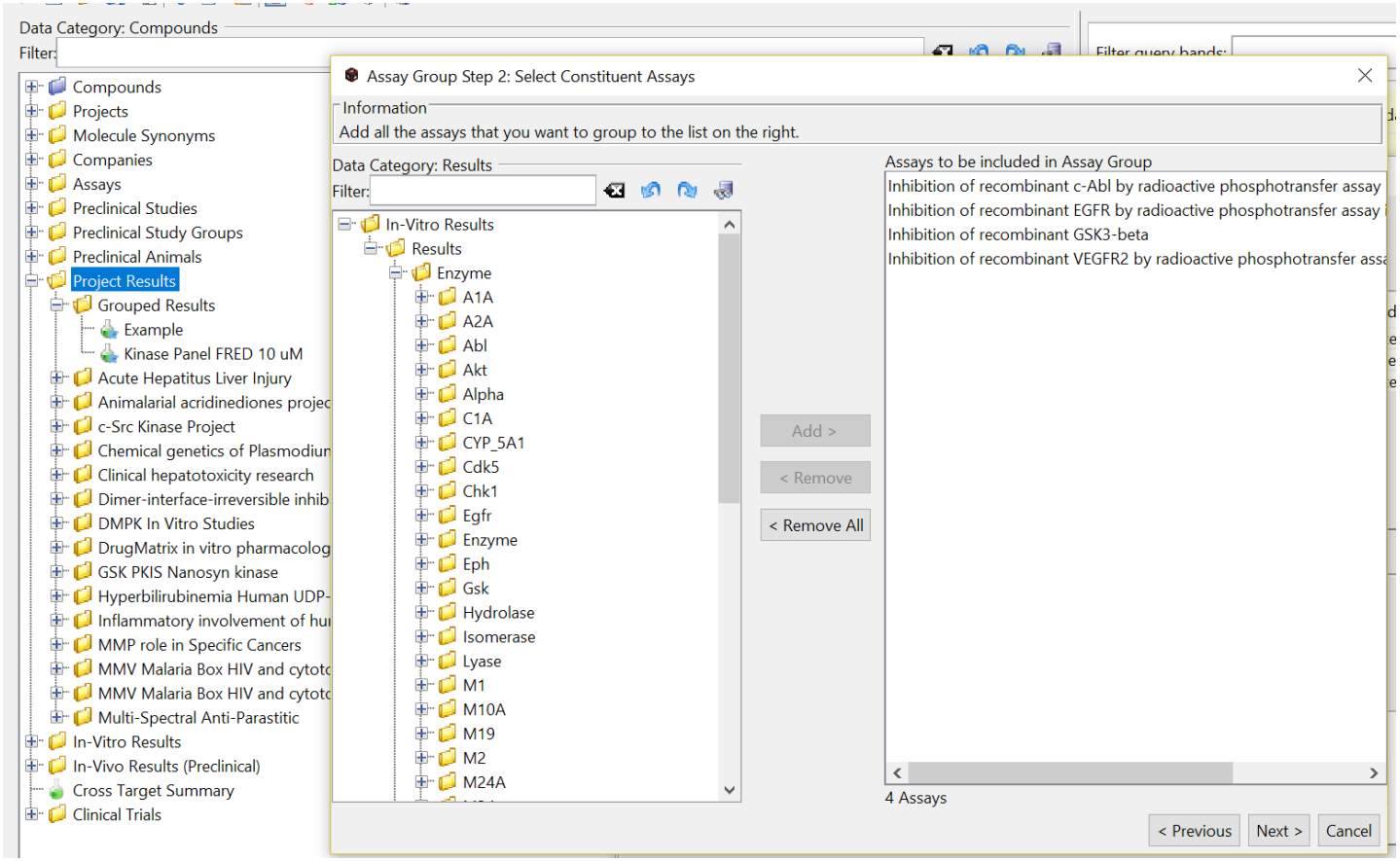
The Evergreens: Super Assays & Assays Groups

- An Assay Group is a “fake” assay that allows retrieval of the results of multiple assays much more easily and keeps the results from individual assays separate



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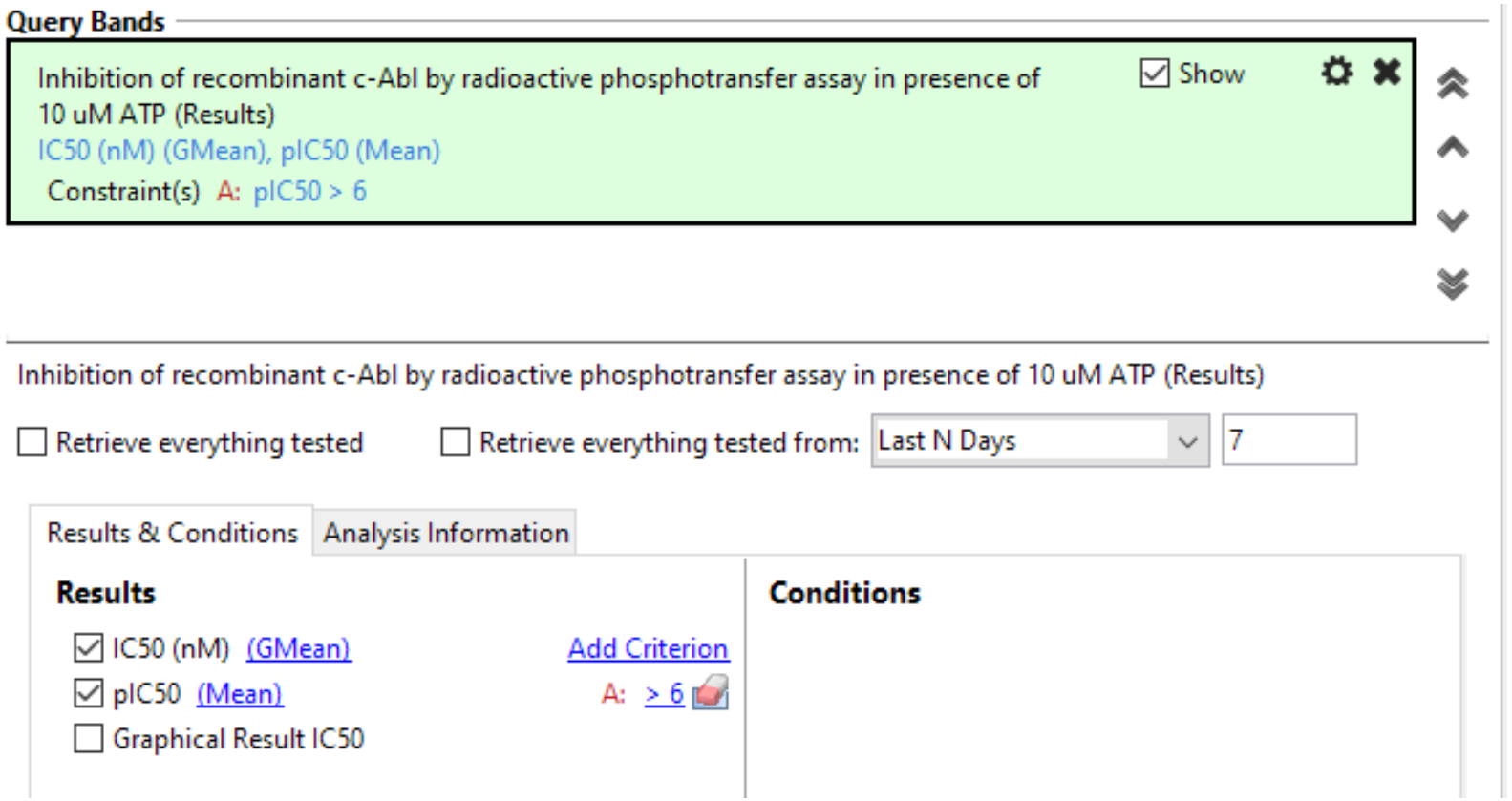
NKOTB - Negative log Results

- Negative log Results



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NKOTB - BioProfile Summary

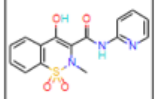
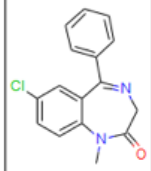
- Most important assay results for all the assays that a compound has been tested in using a compact table representation.

Concatenated Aggregation, Result Type, Unit

Concatenated Condition Names

Concatenated Condition Values (same order as the concatenated Condition Names)

Spreadsheet

	ChEMBL Id	Structure	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:	CHEMBL527		33	Inhibition of human Prostaglandin G/...	Mean Inhibition (%)	-7.000	1	Dose (ug/mL) : Enzyme sub-type	0.1 : PGHS-1
			33	Inhibition of human Prostaglandin G/...	Mean Inhibition (%)	25.000	1	Dose (ug/mL) : Enzyme sub-type	0.1 : PGHS-2
			33	Inhibition of human Prostaglandin G/...	Mean Inhibition (%)	10.000	1	Dose (ug/mL) : Enzyme sub-type	1 : PGHS-1
			33	Inhibition of human Prostaglandin G/...	Mean Inhibition (%)	58.000	1	Dose (ug/mL) : Enzyme sub-type	1 : PGHS-2
			33	Inhibition of human Prostaglandin G/...	Mean Inhibition (%)	35.000	1	Dose (ug/mL) : Enzyme sub-type	10 : PGHS-1
			33	Inhibition of human Prostaglandin G/...	Mean Inhibition (%)	62.000	1	Dose (ug/mL) : Enzyme sub-type	10 : PGHS-2
2:	CHEMBL12		20	Inhibition of [3H]-Ro-15-1788 binding...	Mean Ki (nM)	6.600	1	Receptor sub-type	alpha-2-beta-3-gamma-2
			20	Inhibition of [3H]-Ro-15-1788 binding...	Mean Ki (nM)	13.000	1	Receptor sub-type	alpha-1-beta-3-gamma-2
			20	Inhibition of [3H]-Ro-15-1788 binding...	Mean Ki (nM)	33.000	1	Receptor sub-type	alpha-3-beta-3-gamma-2
			20	Inhibition of [3H]-Ro-15-1788 binding...	Mean Ki (nM)	11.000	1	Receptor sub-type	alpha-5-beta-3-gamma-2
			28	Binding affinity to human recombina...	Mean Ki (nM)	> 3000.000	1	Receptor sub-type	alpha-6-beta-3-gamma-2
			28	Binding affinity to human recombina...	Mean Ki (nM)	14.000	1	Receptor sub-type	alpha-1-beta-3-gamma-2
			28	Binding affinity to human recombina...	Mean Ki (nM)	20.000	1	Receptor sub-type	alpha-2-beta-3-gamma-2
			28	Binding affinity to human recombina...	Mean Ki (nM)	15.000	1	Receptor sub-type	alpha-3-beta-3-gamma-2
			28	Binding affinity to human recombina...	Mean Ki (nM)	11.000	1	Receptor sub-type	alpha-5-beta-3-gamma-2
			10021	Half-maximal inhibition of [125I]-CCK...	GMean IC50 (nM)	> 100000.000	1		
			10022	Half-maximal inhibition of [125I]-CCK...	GMean IC50 (nM)	> 100000.000	1		
			10058	Inhibition of binding of Batrachotoxin...	Mean Inhibition (%)	15.200	1		

Test ID

Test Name

Aggregated Value

Number of values used for aggregation

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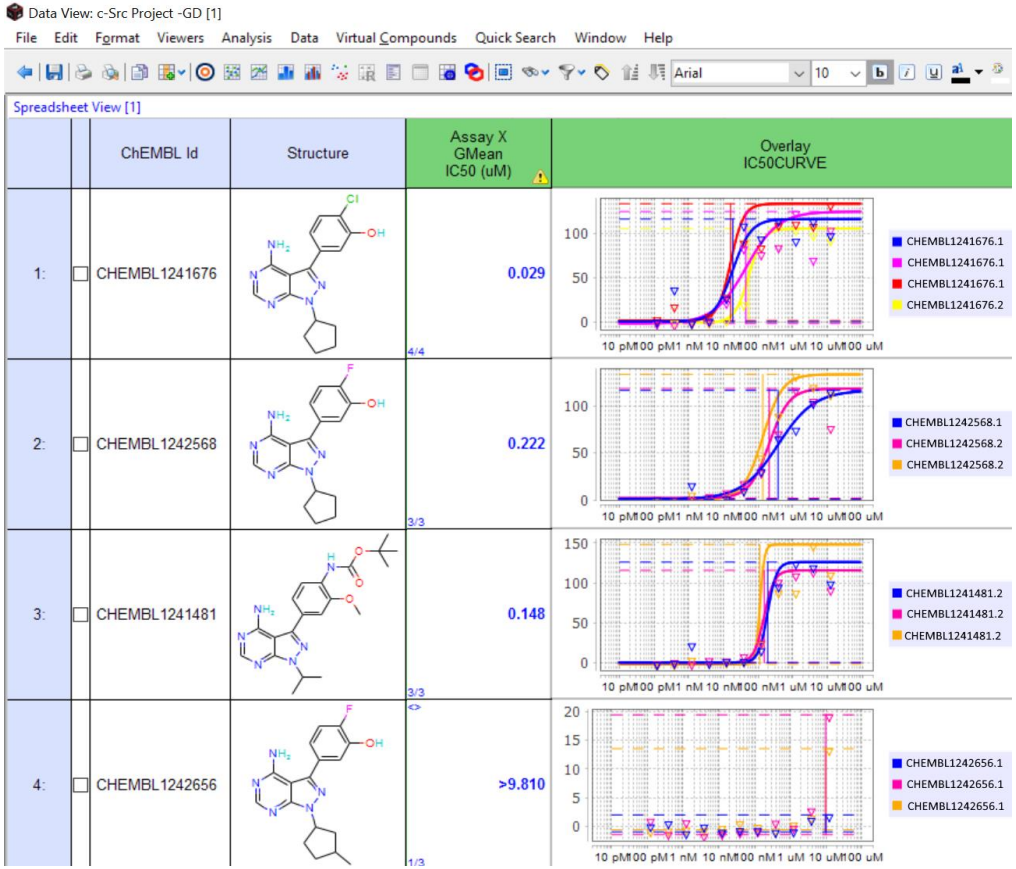
Dose-response curves rendering

- Curve renderer that reproduces fitted dose response curves from result parameters



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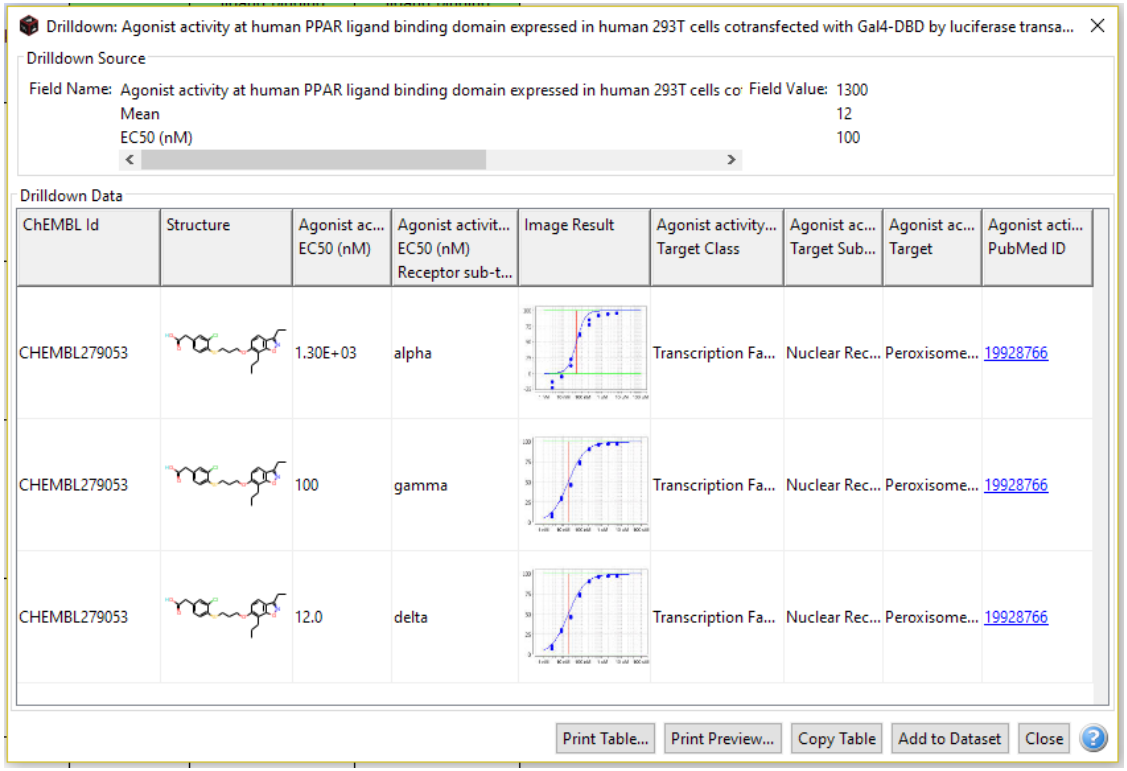
Drilldown templates

- Default drilldown table content can be modified and extended.
  - Change order of columns
  - Pull in additional result types & data fields



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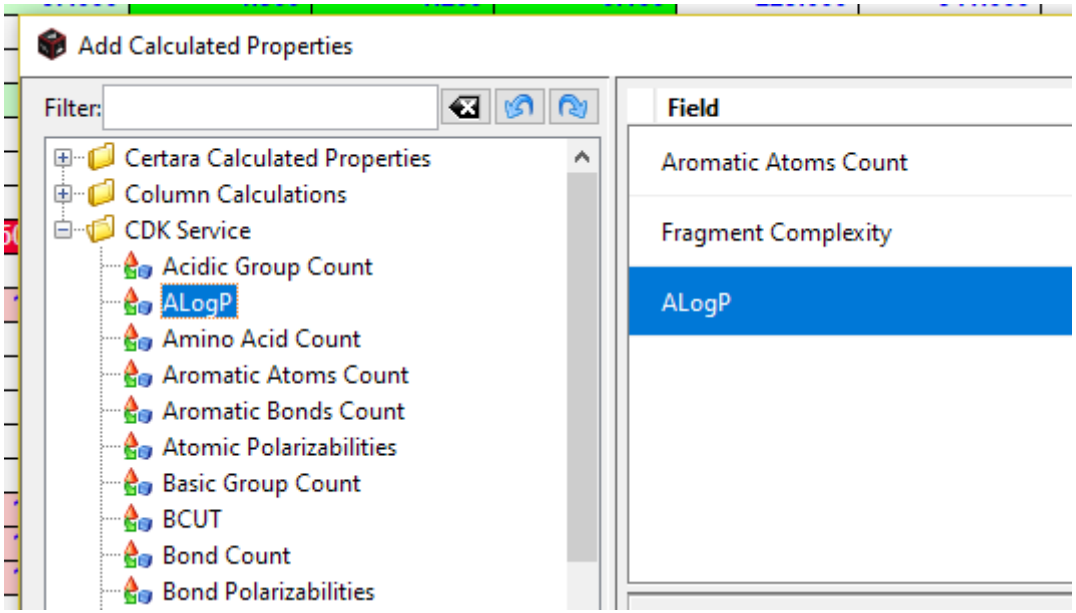
Web Services

Integration with Web Services

- Direct integration into D360 client
  - Property calculations
  - Compound lookup
  - Support for async. and sync. services.



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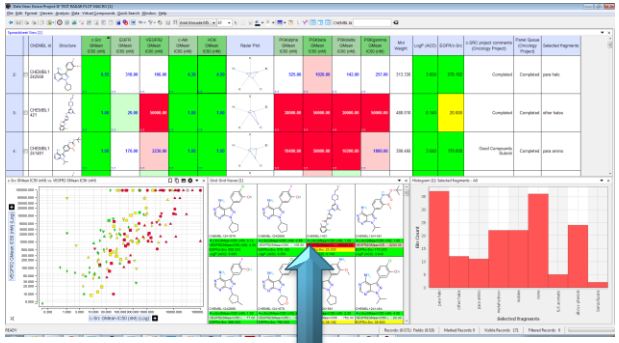
Calculation Caching Server



Applications

Calculation Server

Cached Results

Pipeline Pilot Connector

Asynchronous models or services

Job Management

Synchronous models or services

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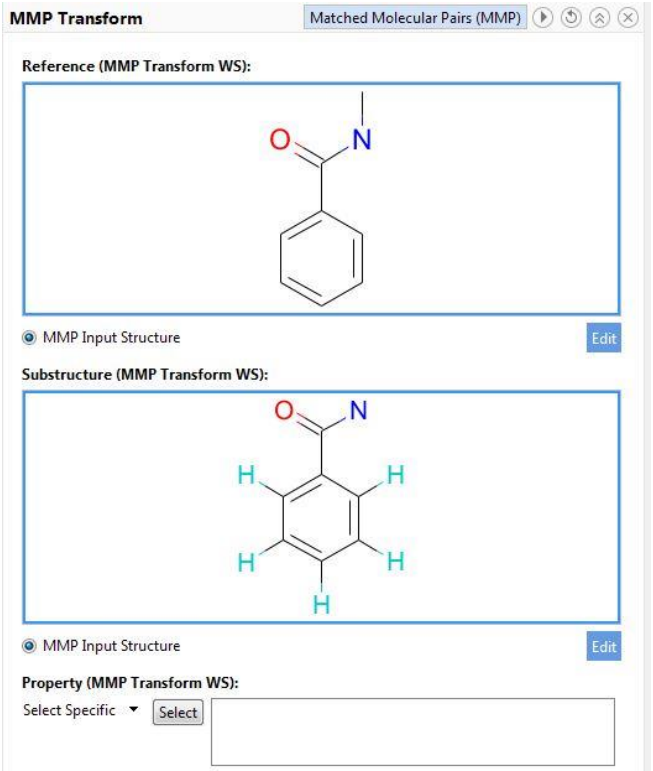
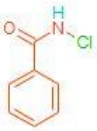
Web Services as Data Source in D360

- Web services can be configured to some extend to act like a virtual database table/view in D360's middle layer.
  - A search within such a virtual table leads to a web service call.
  - Example: Matched Molecular Pair workflows



		Product	Count Property	Delta Property	Sigma Property	SMILES_from Property	SMILES_to Property
1:			1594 1/1	0.211 1/1	0.402 1/1	—R1	Cl-R1
2:			1144 1/1	-0.153 1/1	0.388 1/1	—R1	F--R1

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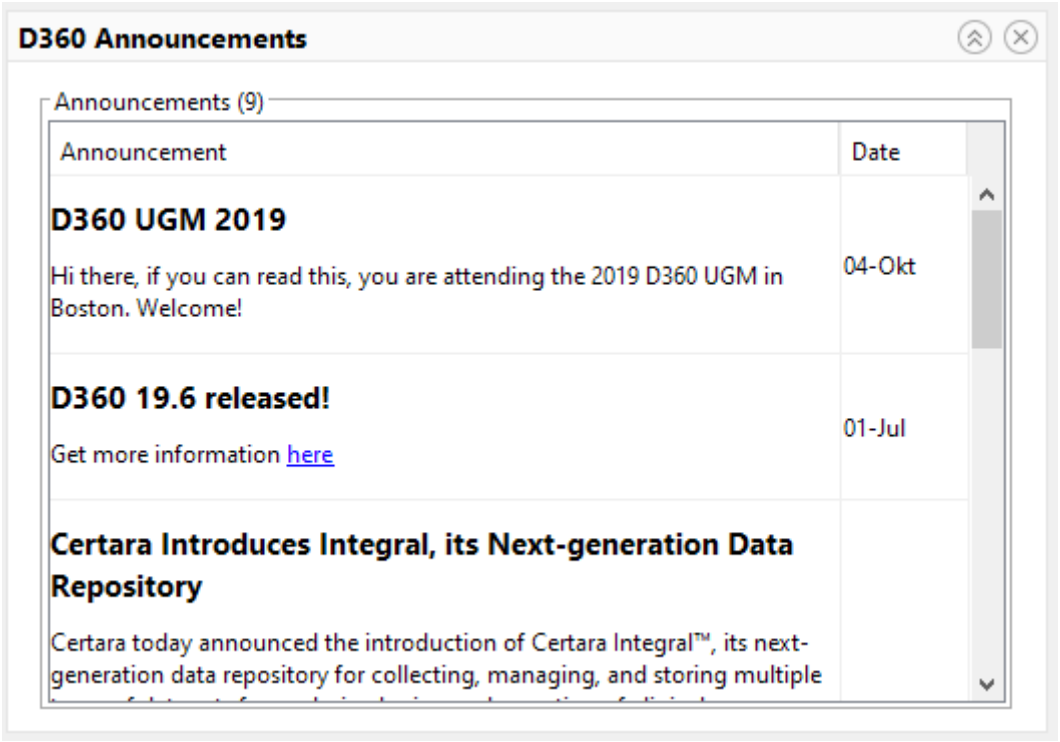
Usability & Security

Announcement/News widget

- Database-backed announcement widget displaying the last n announcements to users.



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Usability & Security

- Interfaces to manage research projects in D360
- TLS encrypted traffic D360 client-server
- Restricting access to data

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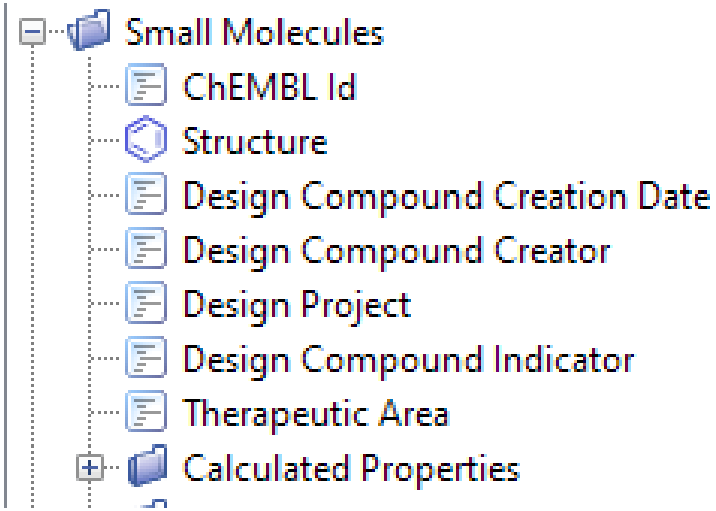
Chemistry

Integration with Virtual/Design Compounds

- Existing virtual compound repository data can be integrated into the standard “Compound” data category such that:
  - Standard queries can retrieve both real and captured virtual compounds.
  - Additional data can be stored about virtual compounds using D360’s annotation system



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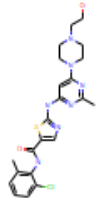
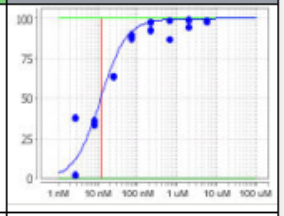
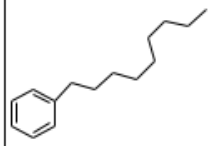
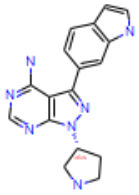
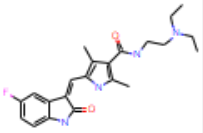
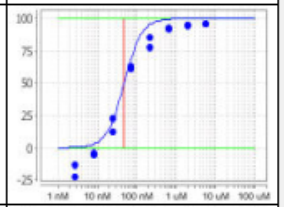
Integration with Virtual/Design Compounds

Spreadsheet

		ChEMBL Id	Structure	Design Compound Indicator	c-Src project comments (Oncology Project)	c-Src Mean IC50 (nM)	c-Src Mean pIC50	c-Src Graphical Result IC50
1:	☐	CHEMBL1421		N	Completed	1 1/1	9 1/1	
2:	☐	DC~00011147		Y	Not interesting			
3:	☐	DC~00011143		Y	Prioritize for synthesis			
4:	☐	CHEMBL535		N	Sutinib;Submit	400 1/1	6.40 1/1	

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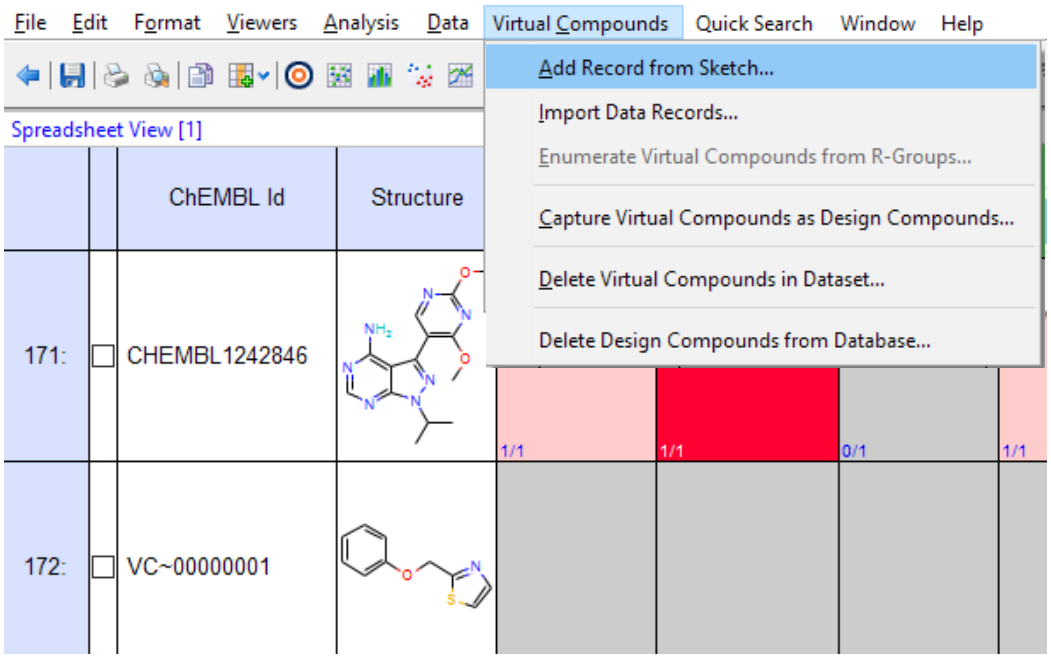
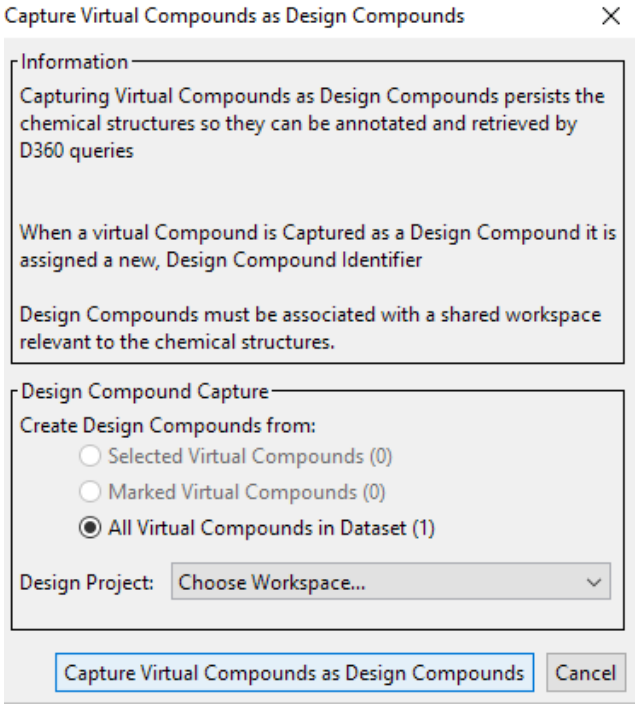
Capturing Compound Ideas

- A D360 dataset may contain real and virtual compounds
  - Sketched into the dataset or imported from a file.

- D360 Capture allows virtual compounds in the dataset to be captured as design ideas.





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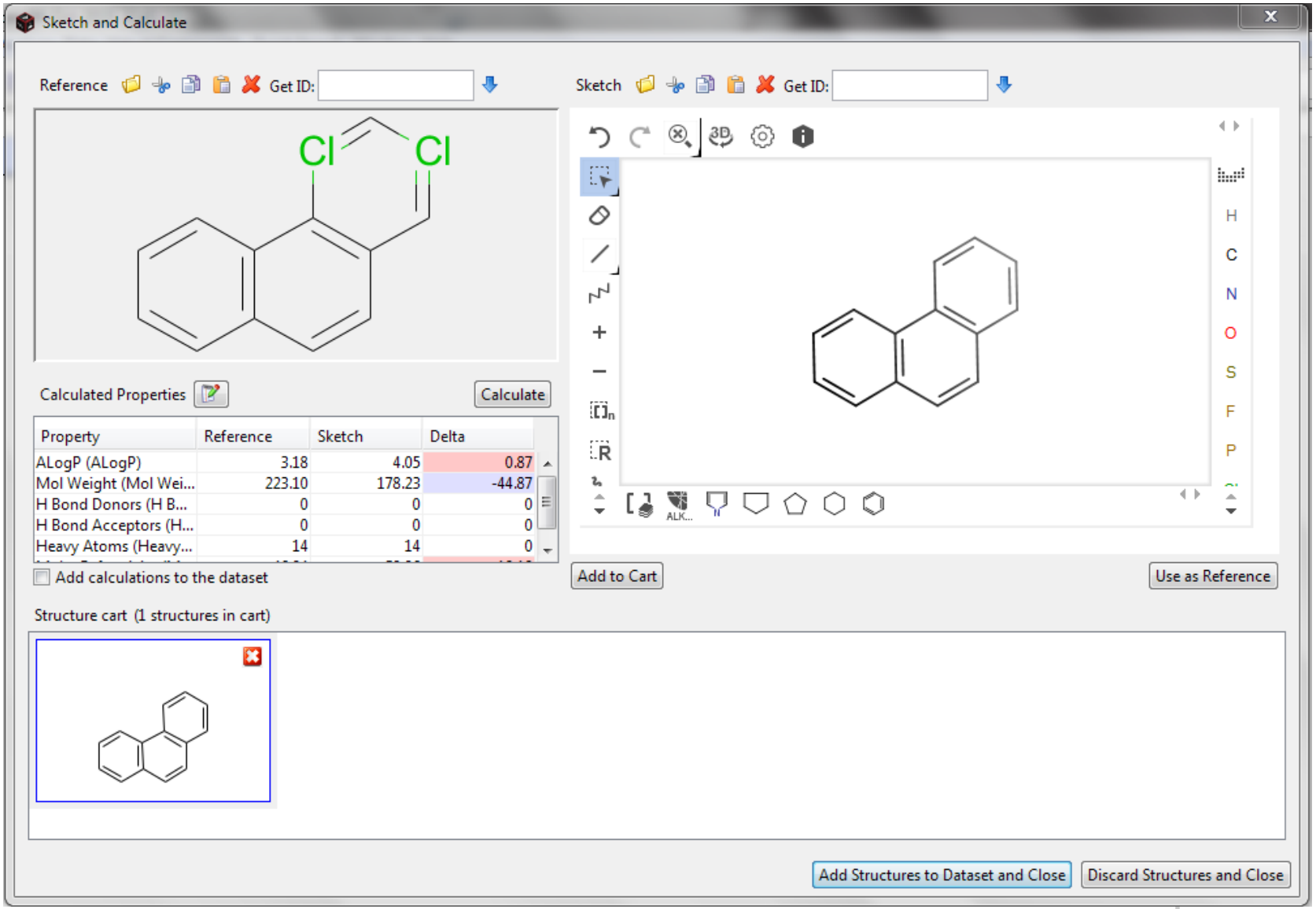
Custom Sketch & Calculate interface



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And so ends our story …

- Wait … are there more stories you can tell? Yes, of course:
  - Custom follow on actions, involving scripting and widget-like interfaces
  - Custom menu entries and right click menus, such as an assay lookup facility
  - Plugins that fetch structures from extra databases for firewalled projects based on the user id
  - …

- The D360 services team is at your disposal to entertain you with more stories of 1001 configurations and help you to bring them to life in your D360 environment.