



**D360**  
**Solving the data access problem**

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## Our Mission

*Enable superior drug development and patient care decision-making*

*through model-informed drug development, regulatory science, real world evidence and knowledge integration,*

*thus optimizing R&D productivity, commercial value and patient outcomes*



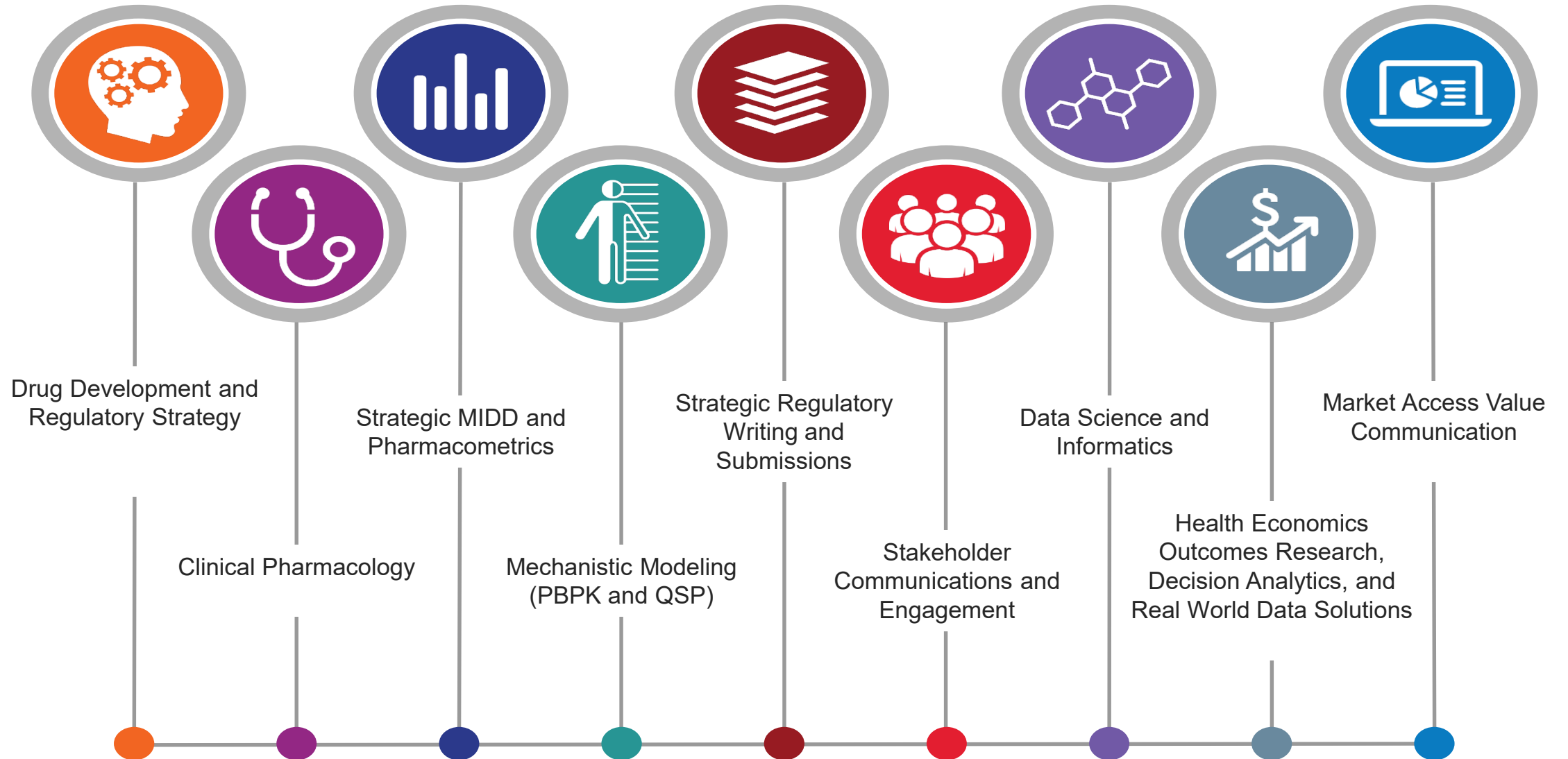
Certara software is used by major regulatory agencies and considered a “gold standard” by the US FDA

# 90%

of all novel drugs approved by the US FDA in the past 3 years were supported by Certara software or services



# Certara's Capabilities



# D360 – Scientific Data Query and Analysis Application

- D360 provides scientists self-service data access to facilitate faster time to insight
- Across different domains
  - Small molecule discovery
  - Biologics discovery
  - Pre-clinical safety
- For a wide range of research organizations
  - 5 of the top 10 pharmaceutical companies
  - Mid-sized biopharmaceutical
  - Small / startups down to ~10 users



# Getting users to their data

**Oncology Project Weekly Screening View** Personal

[Open Query](#)

**Project Data View** Personal

Design Project:  
 Select Specific 

- Antiviral Project
- Oncology Project**
- Osteoarthritis Project

[Open Query](#)



**Data View: Oncology Project Weekly Screening View [1]**

File Edit Format Viewers Analysis Data Virtual\_Compounds Quick Search Window Help

Spreadsheet

	ChEMBL Id	Structure	R1	Mol Weight	c-Src GMean IC50 (nM)	EGFR GMean IC50 (nM)	VEGFR2 GMean IC50 (nM)	c-Abl GMean IC50 (nM)	HCK GMean IC50 (nM)	ALogP	Polarizability	TPSA	Selected fragments	Frequency frags	Ranking frags	Panel Queue (Oncology Project)
1:	CHEMBL1241680		R1	296.300	1500.00	100000.00	4300.00	3400.00	1000.00	3.119	31.979	93.410	para halo other halos	1	16	
2:	CHEMBL1242573		R1	311.320	103.00	1200.00	215.00	87.00	76.00	2.642	34.687	98.300	indoles other halos	1	16	
3:	CHEMBL1242661		-R1	319.360	2400.00	21000.00	550.00	15000.00	540.00	3.280	38.125	78.850	6,6 aromatic alkoxy phenyls	1	16	<input type="button" value="Submit"/>

**Data View: KinaseOrm [1]**

File Edit Format Viewers Analysis Data Virtual\_Compounds Quick Search Window Help

Form: KinaseOrm [1] Structure Similarity Map [1]: Structure All

Zoom: 100%

Project Assays Analytic Data DMPK

c-Src Inhibition GMean, IC50 (nM) # 1,000

Secondary Screens: GMean IC50 (nM) / Selectivity vs c-Src

Assay	GMean IC50 (nM)	Selectivity
EGFR	100000	2380.95
VEGFR2	100000	2380.95
c-Abl	560	13.452
HCK	710	17.000
PI3Kalpha	100000	2380.95
PI3Kbeta	100000	2380.95
PI3Kdelta	1100	25.476
PI3Kgamma	100000	2380.95

ID CHEMBL1241482 Series para halo

Basic Properties

MW (Free Base)	402.4
MW (Full)	402.4
PSA	115.9
Acceptors	6
Donors	2
LogP (ACD)	3.6
LogP (ALogP)	3.3

Advanced Properties

LogD (ACD)	3.3
Rotatable Bonds	4
ROS Violations	0
RO3 Pass	0
Most Acidic PKA	7.7
Most Basic PKA	3.1
Med Chem Friendly	Yes

Off Target Liabilities

Result Type	Mean	Target Class
1	IC50 3.690	Enzyme
2	IC50 0.042	Enzyme
3	IC50 0.565	Enzyme
4	IC50 0.714	Enzyme
5	IC50 1.070	Enzyme

Structure Similarity Map [1]: Structure All

Points closer together represent more similar structures. Points around the edge represent structural outliers.

Filters

Find: 0.120 00000.000

LOG Inhibition of recombinant c-Src by ...

Structure CONTAINS Substructure:

Mol Weight (Free Base) 489.530

Series

- 6,6 aromatic
- Undefined
- alkoxy phenyls
- benzofurans
- indoles
- methoxyhydroxy

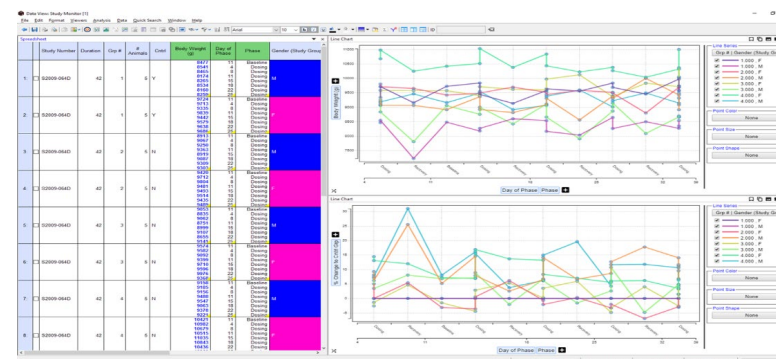
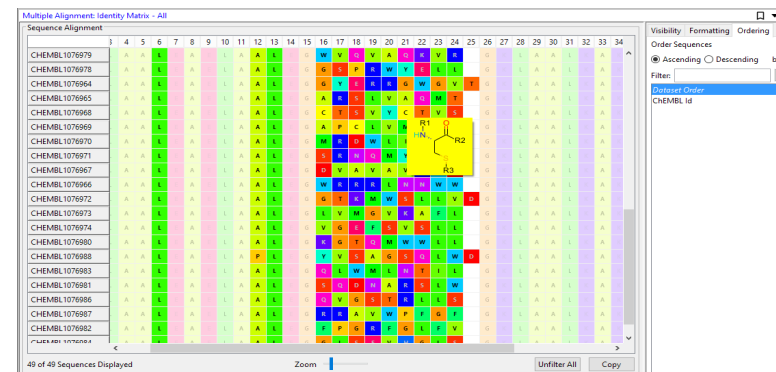
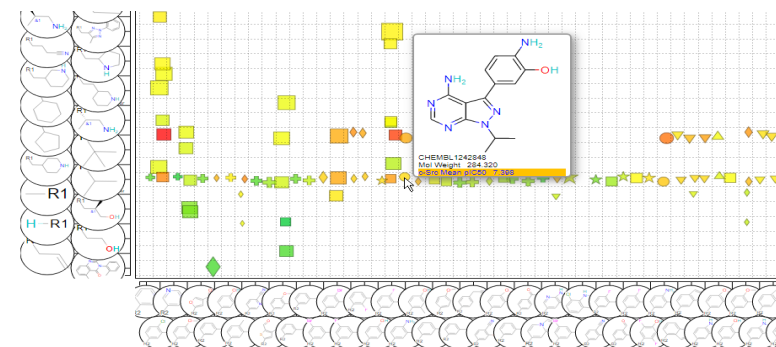
9 of 9 Values Selected

Spreadsheet

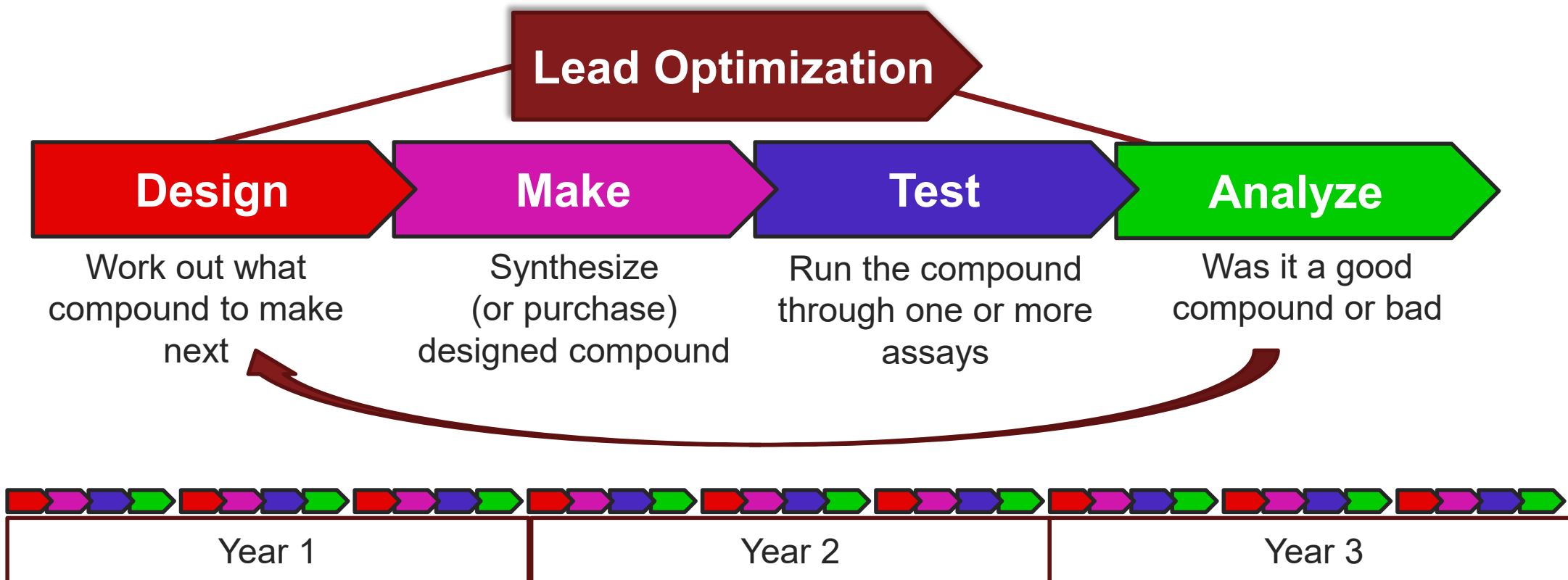
	ChEMBL Id	Structure	c-Src GMean IC50 (nM)	HCK GMean IC50 (nM)	EGFR GMean IC50 (nM)	VEGFR2 GMean IC50 (nM)	c-Abl GMean IC50 (nM)	PI3Ka GMean IC50 (nM)	PI3Kb GMean IC50 (nM)	PI3Kd GMean IC50 (nM)	PI3Kg GMean IC50 (nM)
1:	CHEMBL1241482		42	710	100000	100000	560	100000	100000	1100	
2:	CHEMBL1242207		800	100000	25000	49000	32000	100000	100000	3400	
3:	CHEMBL1241856		130	1100	2700	7200	7900	100000	100000	6000	
4:	CHEMBL1241391		500000	13000	100000	100000	50000	50000	100000	100000	
5:	CHEMBL1242965		23000	10000	45000	10000	14000	100000	52000	22000	
6:	CHEMBL1242751		500	730	3700	5300	11000	10000	100000	37000	
7:	CHEMBL1242960		70	96	5100	10000	830	100000	100000	1900	
8:	CHEMBL1241863		7200	2700	6700	100000	35000	100000	15000	100000	
9:	CHEMBL1242863		2100	1600	100000	100000	2000	15000	100000	1800	
10:	CHEMBL1242757		97	4900	1500	8600	2400	9800	4500	2000	

# D360 Solutions in Different Data Domains

- Small molecule discovery
  - Compound prioritization
  - Compound design
- Biologics discovery
  - Antibodies
  - ADCs
  - Oligonucleotides
  - Peptides
- Preclinical / non-clinical safety
  - Ongoing study monitoring
  - Cross-study data mining



# A Key User Workflow: Design-Make-Test-Analyze



- Shortening the cycle time means you fit more cycles into a year and get to market faster.
- Improving the quality within a cycle means less cycles are required to reach a given point and get to market faster.

# Expanding D360 Applicability



## **Faster Time to Insight**

Data Access, Analysis and collaborative research  
Self-service data access from multiple data sources



***Express***

## **D360 for smaller customers**

Lower price point  
< 40 users, no API access, <=3 data sources



***Partner***

## **D360 for external collaborators**

D360 (or Express) add on  
Easy to set up, secure data access for external research partners



- ChemAxon and Certara have many common customers who successfully integrate ChemAxon and D360 products in their research IT landscape.
- Integration with ChemAxon tools include:
  - JChem Cartridge, to provide chemical structure searching within data queries.
  - Compound Registration, works as data source for D360.
  - Marvin Sketch, can be used with D360 for structure input.
  - Custom compound sketcher created for one customer using MarvinJS.
  - Marvin Live, under investigation.