



D360
Solving the data access problem

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22 May, 2019

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



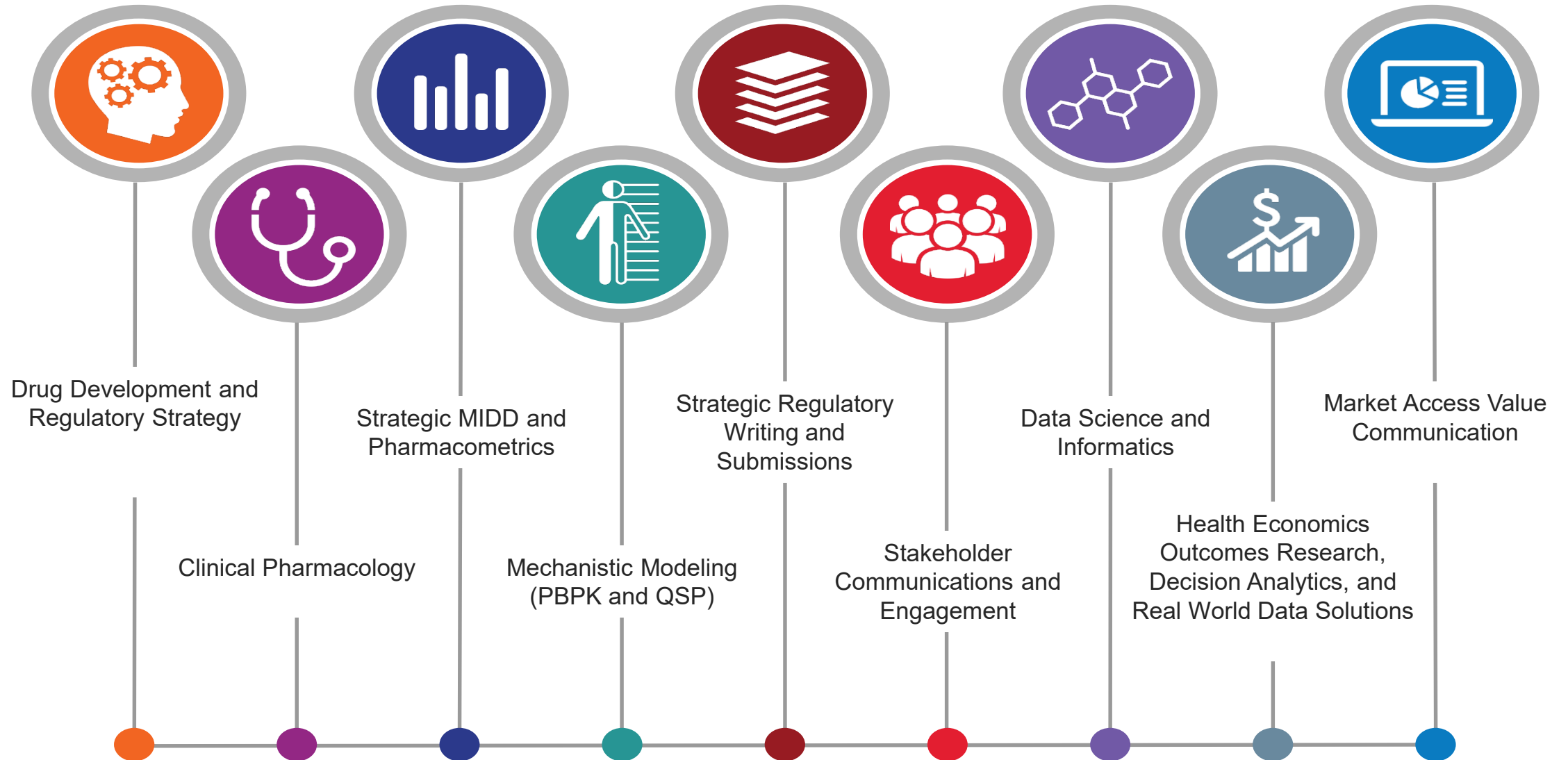
Certara software is used by major regulatory agencies and considered a “gold standard” by the US FDA

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

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	13452
HCK	710	17000
PI3Kalpha	100000	2380.95
PI3Kbeta	100000	2380.95
PI3Kdelta	1100	25476
PI3Kgamma	100000	2380.95

Structure Similarity Map [1]: Structure All

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

Filters

LOG Inhibition of recombinant c-Src by ...

Mol Weight (Free Base)

Series

- 6.6 aromatic
- Undefined
- alkoxy phenyls
- benzofurans
- indoles
- metahydroxy

9 of 9 Values Selected

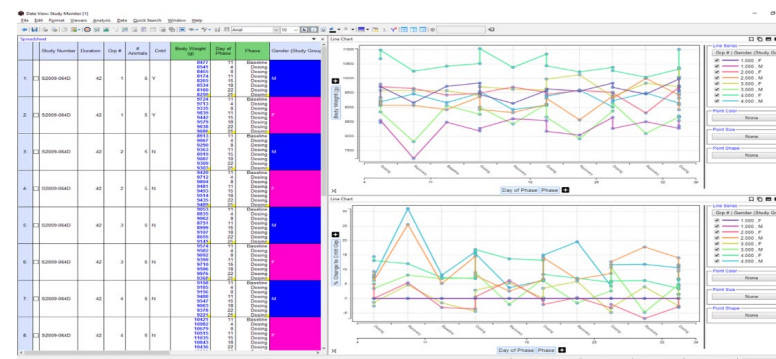
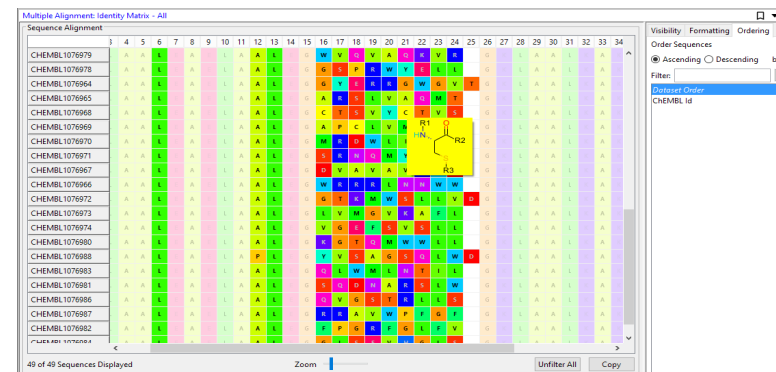
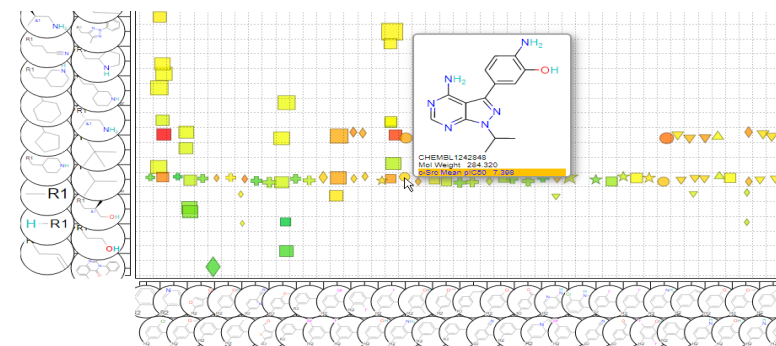
Spreadsheet

	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	10000	52000	22000	
6:	CHEMBL1242751		500	730	3700	5300	11000	10000	10000	37000	
7:	CHEMBL1242960		70	96	5100	10000	830	10000	10000	1900	
8:	CHEMBL1241863		7200	2700	6700	10000	35000	10000	15000	10000	
9:	CHEMBL1242863		2100	1600	10000	10000	2000	15000	10000	1800	
10:	CHEMBL1242757		97	4900	1500	8600	2400	9800	4500	2000	

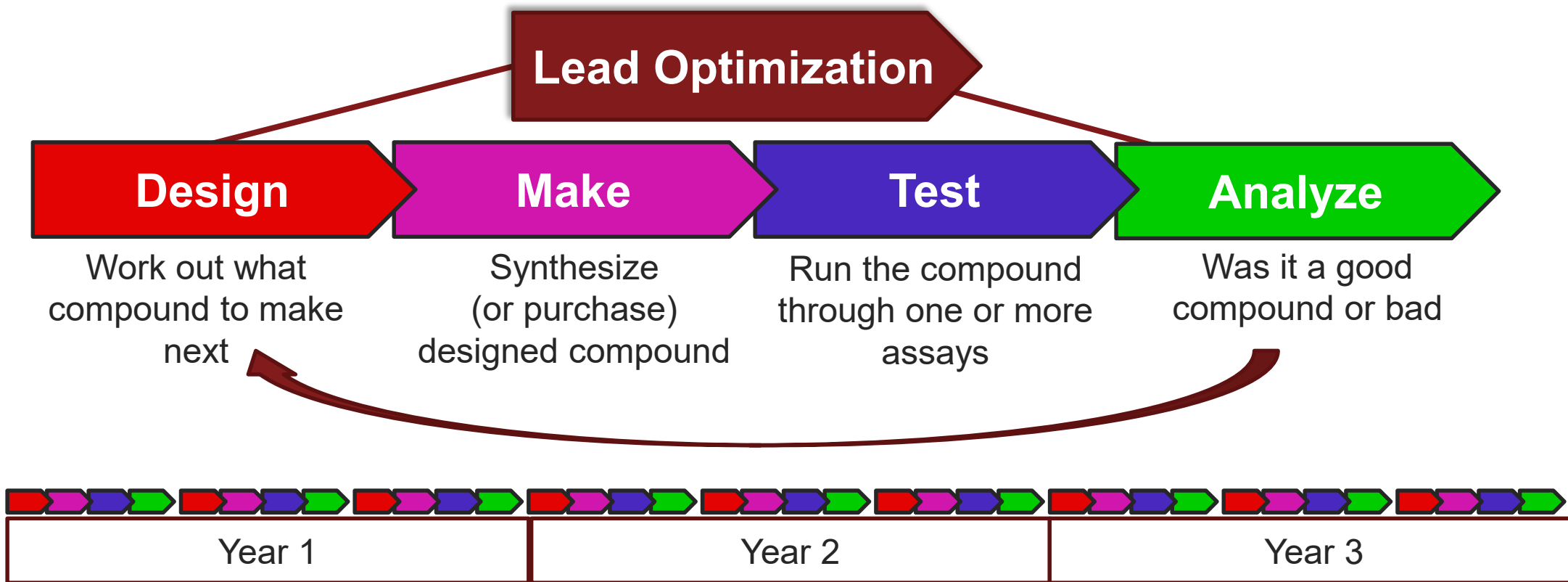
Histograms: Histogram [1]: Inhib... Histogram [2]: Inhib... Histogram [3]: Inhib... Histogram [4]: Inhib... Histogram [5]: Inhib... Histogram [6]: Inhib... Histogram [7]: Inhib... Histogram [8]: Inhib... Histogram [9]: Inhib...

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.