

D360™ Scientific Informatics Platform for Drug Discovery and Development



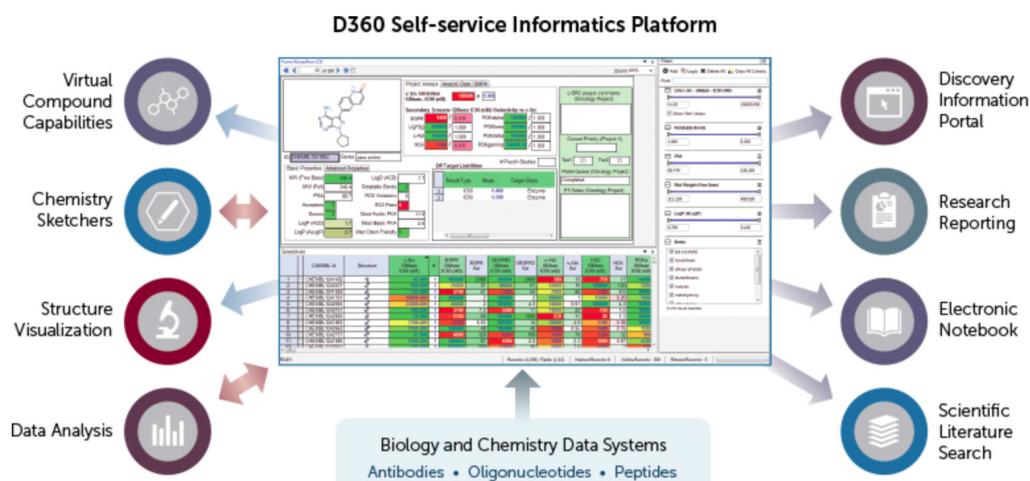
D360 ▪ D360 Express ▪ D360 Capture ▪ D360 Partner ▪ Pre-clinical Safety Storage

D360™ is the industry-leading scientific data informatics hub used globally by over 6,000 discovery research scientists for small molecule and biologics discovery and pre-clinical translation. It was designed to meet the discovery researcher's workflow by providing a self-service data access and integrated analysis solution. Focus your R&D expertise on data understanding, versus time-consuming data assembly.

Solutions to Meet All Needs: From Small Biotech to Large Global Pharma

Drug discovery and development requires the understanding of complex chemical, biological, logistical, and computational data from a wide variety of data sources. Whether you access data from a single source or require a more comprehensive enterprise solution for data integration, D360 toolkits and add-on products provide the flexibility to choose the solution that is optimized for your organizations' needs resulting in high fidelity data access for fast, effective go/no-go decisions and faster time to insight. Simplified deployment, expandability, and easy administration enables a wide-range of customizable capabilities to support collaboration across teams and external research partners.

The D360 user desktop hub provides an intuitive interface for self-service data access and analysis - with a few simple clicks, queries can be created or executed that retrieve, transform, and present the data in the required format for analysis, without any manual data manipulation or dedicated IT support, and regardless of where and how the data is stored.



Capabilities That Go Beyond Data Retrieval

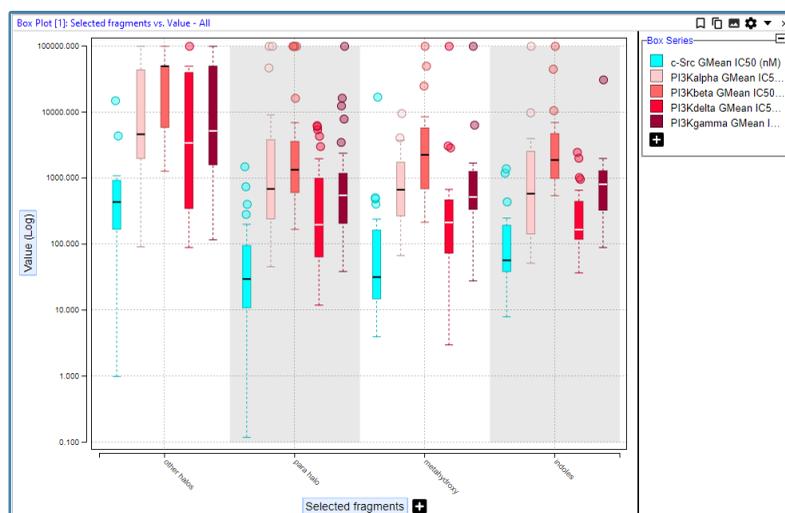
Interactive data filtering, exploration, and numerous visualizations provide built-in analysis and calculation of key parameters.

- Histograms, bar, and box charts allow simple comparison of experimental and calculated result profiles across groups of tested entities
- Dose-curve rendering reproduces fitted dose-response curves from result parameters enhancing the understanding of data qualities and extends D360's abilities to satisfy biologists' workflows
- The Bioprofile Summary Data View provides visualization of how a substance has acted in all the assays it has been tested

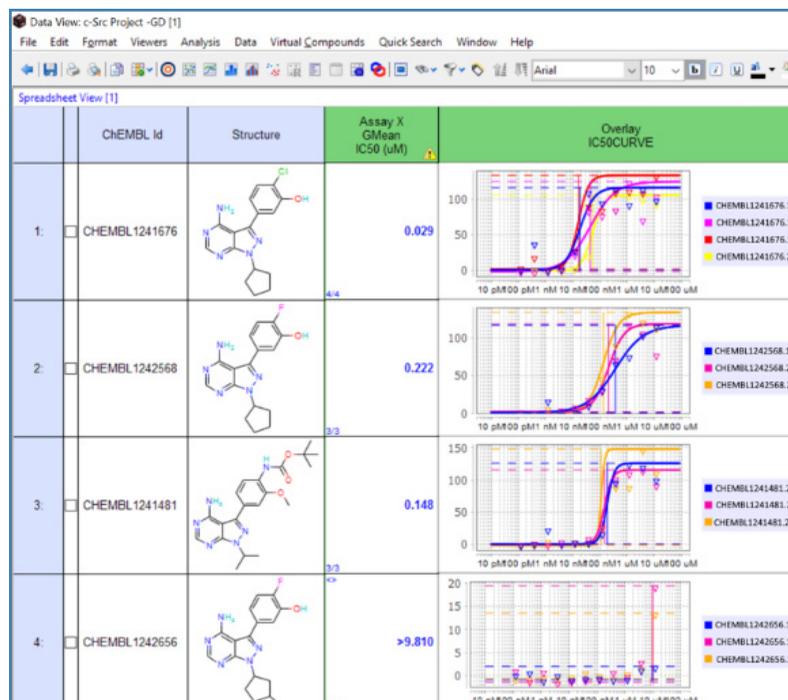
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D360 is the core gateway for us in accessing information, it's the flexibility and extensibility that we were looking for. D360 really does allow us to evolve and grow, as our R&D teams are changing the way they work rapidly to find innovative approaches to drug discovery.

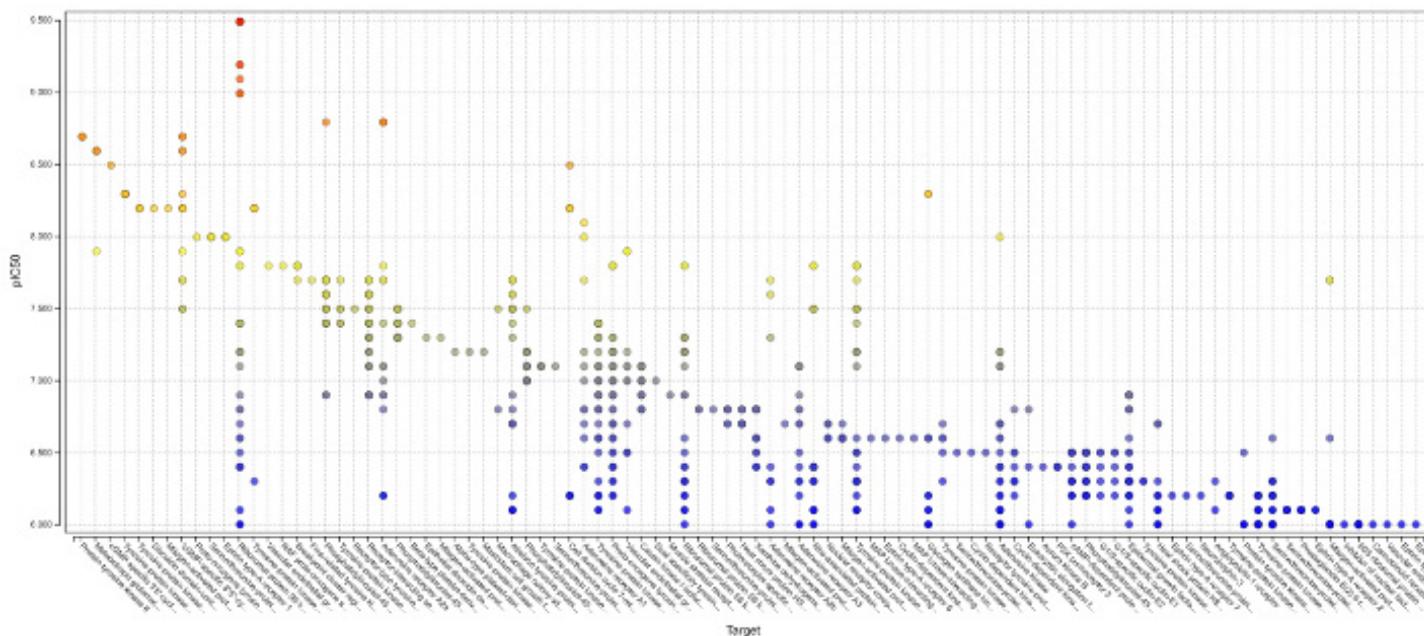
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Box chart displaying assay activity distribution for primary (cyan) and selectivity assays (red) of the five best chemical series



Dose-response curve visualization from multiple experimental runs



The Bioprofile Summary View displays only those principal compound test results that have been identified via configuration to be the most important for each assay, utilizing the default aggregation function for each identified result type.

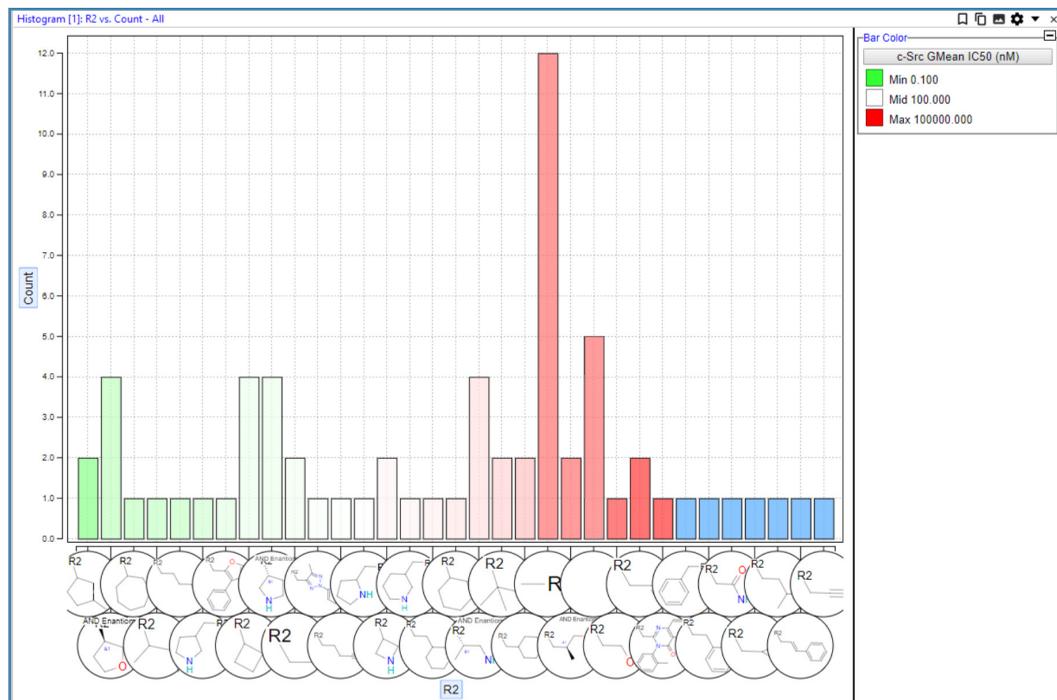
D360 Toolkits for Data Design, Access, and Analysis of Multiple Modalities

Drug discovery and development projects evaluate a range of modalities as potential therapeutic agents such as small molecules and biologics including oligonucleotides, antibodies, peptides, proteins, and antibody-drug conjugates. The representation of these entities and the research processes required to test them as prospective treatments for a wide range of disease areas vary widely. D360 provides the ability to quickly access, understand, and share data with toolkits for small molecule discovery, biologics discovery, and pre-clinical translation - each tailored to meet specific research goals.

D360 Small Molecule Discovery Toolkit

The D360 Small Molecule Discovery Toolkit provides embedded SAR Analysis and Molecular Design Tools, including R-group analysis, chemical series, and matched series analysis which can be leveraged for comprehensive design and analysis of small molecules.

- Matched Molecular Series Analysis (MMS) examines specific sites of variation in chemical structures and their effect on molecular property profiles
- Structure Comparison Viewer provides side-by-side comparison of two chemical compounds and their associated data
- Virtual Compound provides the capability to use the output of R-Group Analysis to enumerate virtual structures to fill in the R-Group matrix – virtual structures created through enumeration can be analyzed alongside real structures to make decisions on the forward path for the project



Histogram visualization of R2 substituents from an R-group analysis by value and axis structures

D360 Biologics Discovery Toolkit

D360 Biologics Discovery Toolkit enables medically-relevant sequence alignment and analysis for oligonucleotides, peptides, antibodies, and antibody-drug conjugates. Enhanced functionality for sequence-activity relationships of biologics helps users optimize biologics modalities by deriving sequence activity relationships.

Oligonucleotides

D360 provides capabilities for improved understanding of the relationship between the composition of oligonucleotides and their biological profile. Using HELM nomenclature searchability, filtering and similarity calculations can be done on oligonucleotides represented either by a single sequence (base) or by multiple related sub-sequences. Formatting of oligonucleotide sequences allows sequence activity relationships to be uncovered.

- Search oligonucleotides by composition and similarity
- Display oligonucleotide sequences and sub-sequences
- Format sequences based on their own composition or the composition of a related sub-sequence at aligned positions

Multi-Parameter Optimization

The key difficulty in any therapeutic program is the ability of scientists to modify the candidate substances they are developing to generate the biological profile that is expected to lead to a new medicine. By providing a flexible scoring function that can take all relevant parameters into account and balance them against each other, the best candidates with a desirable property profile can be identified more quickly and effectively.

Multi-parameter scoring allows candidate medicines to be scored according to all-important properties that affect the likelihood of becoming a valuable therapeutic agent.

Smearhead View [1]	CHEMBL ID	Structure	1-2h Oblam pIC50 (nM)	3-24h Oblam pIC50 (nM)	10-24h Oblam pIC50 (nM)	LD50 Oblam pIC50 (nM)	PKC Oblam pIC50 (nM)	PKA Oblam pIC50 (nM)	PKB Oblam pIC50 (nM)	PKC Oblam pIC50 (nM)	PKA Oblam pIC50 (nM)	PKB Oblam pIC50 (nM)	PKC Oblam pIC50 (nM)
1	CHEMBL1241676		8.5	67	4.3	1.3	8.16	229	949	199	199	199	199
2	CHEMBL1242048		8.5	326	189	4.3	4.3	129	199	149	209	199	199
3	CHEMBL1241		8.5	25	20000	1	1	2000	1000	2000	1000	1000	1000
4	CHEMBL1242048		8.5	326	77	6.4	5.7	250	139	6.7	239	199	199
5	CHEMBL1241676		8.5	1199	68	21	8.8	119	199	21	139	199	199
6	CHEMBL1242042		8.5	271	59	49	19	199	199	62	279	199	199
7	CHEMBL1241444		8.5	149	29	5.2	1	149	49	5.2	199	199	199
8	CHEMBL1242048		8.5	449	19	31	5.1	399	139	31	499	199	199
9	CHEMBL1242798		8.5	179	49	24	4.4	279	349	24	179	199	199
10	CHEMBL1242042		8.5	449	299	59	19	69	299	59	449	199	199

Sorted by primary activity:
top compounds have poor profile
(many bad/red values)

Sorted by multi-parameter score:
top compounds have a desirable overall profile
(many desirable/green values)

Protein and Peptide Sequence Capabilities

Knowledge extracted from aligned peptide sequences and short protein segments is used for rational design, focusing on the monomers and motifs responsible for desired biological activity profiles. Peptide sequences can be aligned and color-coded by property, while areas of sequence difference can be highlighted. This provides sequence analysis capabilities that can help users derive sequence-activity relationships to optimize bioprofiles.

Peptide Sequence Alignment

Display of experimental data in conjunction with multi-parameter cores provides the sequence-activity relationship. The peptide sequence alignment viewer provides the basis for sequence-activity analysis by aligning sequences either to a reference sequence or to each other:

- Highlight sequence alignments to areas of similarity/difference
- Format to display molecular properties
- Filter residues at a specific aligned position
- Display atomistic level of monomer structures

Multiple sequence alignment of peptide sequences colored by residue property. Mouse-over on a single residue displays the atomistic structure of the monomer.

Multiple Alignment: Identity Matrix - All

Sequence Alignment

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33
CHEMBL1076928	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	E	R	R	L	I	T	F	R	S	G	L	A	A	L	A	L	A	
CHEMBL1076943	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	A	R	H	F	Y	V	S	V	G	L	A	A	L	A	L	A	L	
CHEMBL1076944	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	R	S	F	D	P	V	C	S	W	G	L	A	A	L	A	L	A	
CHEMBL1076941	dA	L	A	A	L	A	A	L	A	L	A	L	A	L	G	W	R	D	P	M	D	S	V	G	L	A	A	L	A	L	A	L	
CHEMBL1076940	dA	L	A	A	L	A	A	L	A	L	A	L	A	L	G	A	R	I	C	C	S	W	G	L	A	A	L	A	L	A	L	A	
CHEMBL1076947	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	L	L	W	H	S	L	W	G	L	A	A	L	A	L	A	L	A	
CHEMBL1076946	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	R	D	Q	V	M	F	L	H	G	L	A	A	L	A	L	A	L	A
CHEMBL1076945	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	L	E	G	K	S	M	G	F	I	G	L	A	A	L	A	L	A	L
CHEMBL1076952	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	S	G	M	L	A	H	F	S	W	G	L	A	A	L	A	L	A	L
CHEMBL1076950	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	N	I	S	R	F	W	V	L	A	G	L	A	A	L	A	L	A	L
CHEMBL1076951	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	Y	E	G	F	M	W	L	I	G	L	A	A	L	A	L	A	L	A
CHEMBL1076948	dA	L	A	A	L	A	A	L	A	L	A	L	A	L	G	lalloT	L	V	V	S	W	D	F	W	G	L	A	A	L	A	L	A	L
CHEMBL1076949	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	W	V	G	M	R	F	V	W	R	G	L	A	A	L	A	L	A	L
CHEMBL1076955	dA	L	A	A	L	A	A	L	A	L	A	L	A	L	G	P	Q	P	M	W	G	S	W	R	G	L	A	A	L	A	L	A	L
CHEMBL1076953	A	L	A	A	L	A	A	L	A	L	A	L	A	L	G	L	I	G	V	L	S	Y	I	F	G	L	A	A	L	A	L	A	L

49 of 49 Sequences Displayed

Zoom | Unfilter All | Copy Alignment

Records: (0/49) Fields: (0/2) | Marked Records: 0 | Visible Records: 49 | Filtered Records: 0

Visibility | Formatting | Ordering

Highlight

- None
- Sequence Identity
- Sequence Difference

Hide

- None
- Sequence Identity
- Sequence Difference

“ D360 provides medically-relevant sequence alignment and analysis versus the traditional bioinformatics techniques which examine evolutionary relationships – a differentiation that is essential in the discovery and development of peptide therapeutics that are not limited to the 20 naturally-occurring amino acids. ”



D360 has drastically reduced the time and resource we spend getting data to all of our scientists, and really enables us to make pivotal decisions in a much more rapid timeframe.



D360 Express

Out-of-the-Box Integrated Self-Service Informatics Solution

D360 Express provides all the functionality for small molecule and biologics data design, access, visualization, and analysis that is contained in D360, however is specifically designed for discovery scientists at smaller pharmaceutical organizations that do not require an enterprise solution for data integration.

Get up and running quickly and affordably

D360 Express comes with standard connectors to your data sources and can be quickly deployed, without changes to your existing IT infrastructure, and with minimal IT support. Connectors are available for data sources from BioVia, Core Informatics, IDBS, PerkinElmer, and more. Customized implementation packages to non-standard data sources are available.

- Connect and integrate chemical and biological data in one central view from commercial data solutions and public databases
- Provide a shared workplace environment for queries, datasets, lists, and comments creating a self-sustaining user community
- Collaborate in real-time in a self-service environment

D360 Capture - Streamlining Design with Virtual Compounds

D360 Capture is an add-on product to D360 that extends the compound design capabilities by allowing the capture of virtual compounds as design compounds for further prioritization. Virtual compounds can be retrieved, analyzed, and annotated alongside real compounds in standard D360 queries to allow for the capture, assessment and prioritization of new design ideas.

D360 Capture adds on to your existing D360 deployment:

- Capture new chemical structure ideas in a centralized repository directly from D360
- Directly integrate captured virtual compounds into existing D360 configuration
- Retrieve both real and design compounds into the same dataset from standard compound queries
- Compare real and design compounds within the same data view, utilizing the same set of analysis tools
- Use D360's annotations to comment on and prioritize design compounds for synthesis
- Augment with additional data, access directly, or via provided web services from outside the D360 application

D360 Partner – Simplify Secure Data Access and Collaboration with Research Partners

D360 Partner is an affordable add-on product for D360 for external partners that allows for seamless, secure sharing of data and analysis while advancing communication and collaboration. D360 Partner provides an alternate D360 client application for external research partners that securely connects them to relevant data from the sponsor's main D360 instance.

- External research partners share the same data views and analysis tools as the sponsor without access to unauthorized data
- Partners and sponsor can share status and ideas through D360 annotations
- Partners can be on-boarded and ramped up and down quickly and easily

D360 Partner provides 3 levels of data security:

1. The D360 data catalog and queries are never available within the D360 Partner client to prevent any unauthorized data access
2. Partners are not allowed to build or adjust data queries or add data to datasets, preventing inadvertent data access by partners
3. Data views are created by the sponsor and provided to external partners as simple D360 Dashboard QuickSearch widgets

Pre-Clinical Safety Store

A CDISC SEND-based Data Repository for Pre-clinical Study Data

Pre-clinical Safety Store (PCSS™) is a queryable repository in which pre-clinical study data can be uploaded, validated and matched for desired terminology based on CDISC SEND standards. When used in conjunction with D360, PCSS is an invaluable tool for study managers, toxicologists, pathologists, and data scientists. The PCSS plug-in architecture takes advantage of existing IT infrastructure, supports diverse file formats, and connects to 3rd party platforms such as Provantis®, Pristima™, and Watson LIMS™.

Make Better Informed Decisions for Discovery and Development of Small Molecules, Biologics and Pre-clinical Translation Studies

D360 Scientific Informatics Platform includes toolkits and add-on products to provide state-of-the-art capabilities that go beyond standard data retrieval platforms. D360 has been deployed across a wide range of companies: from small biotech firms that need data access from a single data source, to large global pharma companies that require a more comprehensive enterprise solution for data integration. Regardless of size and need, D360 demonstrates that simplified data access and integrated data analysis leads to faster time to insight and greater scientific understanding.

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D360 Partner is the perfect solution for sharing the data with our external collaborators.”

About Certara

Certara is a leading provider of decision support technology and consulting services for optimizing drug development and improving health outcomes. Certara's solutions, which span the drug development and patient care lifecycle, help increase the probability of regulatory and commercial success by using the most scientifically advanced modeling and simulation technologies and regulatory strategies. Its clients include hundreds of global biopharmaceutical companies, leading academic institutions and key regulatory agencies.

For more information visit www.certara.com or email sales@certara.com.