

Add Off-target Risk Profiling to Your Analyses

D360™ is Certara's industry-leading scientific informatics platform, designed to help discovery scientists spend more time analyzing leads and less time wrangling data. More than 6,000 scientists across pharma and biotech rely on D360 to integrate experimental, computational, and logistical data into a single intuitive data view from which compounds can be prioritized and new entities designed.

With self-service data access, customizable dashboards and advanced visualization tools, D360 streamlines the Design-Make-Test-Analyze (DMTA) cycle by bringing speed and completeness to the exploration of structure-activity relationships (SAR). The result is quicker, smarter decision-making for both small molecule and sequence-based modalities, including antibodies, peptides, oligos and more without needing a supporting IT department.

Now, D360 is integrated with Certara's **Secondary Intelligence**™ to power off-target risk profiling.

Predictive technology to evaluate risks from off-target interaction

Secondary Intelligence is a risk assessment tool based on secondary pharmacology data. Until now it has been tailored for use by preclinical safety scientists responsible for interpreting secondary pharmacology readouts of small molecule compounds and using the data in risk assessment.

D360 now supports a key feature of Secondary Intelligence: a low-medium-high ranking of the likelihood of clinically concerning receptor modulations. The enhancement expands upon percent inhibition and K_i data inside D360 with an expertly-derived clinical risk assessment for each off-target receptor in a standard screening panel of small molecules. D360 displays this intelligence alongside other assay data and tools for multi-parameter optimization, allowing scientists to iterate on designs informed by a range of properties for each entity.

Now your discovery team can save the time and expense of in vivo studies for leads likely to fail for safety reasons.

Sample Code	Structure	MACHR3 Secondary Intelligence	ADRA2A Secondary Intelligence	CBR2 Secondary Intelligence	DAT Secondary Intelligence	ACHE Secondary Intelligence	CAV1P2 Secondary Intelligence
1 EX00000001		Inh: 31.0 % K _i : 15898.6 (nM)	Inh: 6.0 % K _i : 13333.3 (nM)	Inh: 60.0 % K _i : 4347.8 (nM)	Inh: 16.0 % K _i : 15882.4 (nM)	Inh: 4.0 % K _i : 30000.0 (nM)	Inh: 48.0 % K _i : 2443.4 (nM)
2 EX00000002		Inh: 40.0 % K _i : 10714.3 (nM)	Inh: 52.0 % K _i : 4102.6 (nM)	Inh: 49.0 % K _i : 6787.9 (nM)	Inh: 85.0 % K _i : 934.3 (nM)	Inh: 8.0 % K _i : 30000.0 (nM)	Inh: 84.0 % K _i : 989.0 (nM)
3 EX00000003		Inh: 7.0 % K _i : 21428.6 (nM)	Inh: 11.0 % K _i : 13333.3 (nM)	Inh: 47.0 % K _i : 7354.3 (nM)	Inh: 1.0 % K _i : 15882.4 (nM)	Inh: 7.0 % K _i : 30000.0 (nM)	Inh: 11.0 % K _i : 15576.9 (nM)
4 EX00000004		Inh: -3.0 % K _i : 21428.6 (nM)	Inh: -5.0 % K _i : 13333.3 (nM)	Inh: -13.0 % K _i : 19565.2 (nM)	Inh: 2.0 % K _i : 15882.4 (nM)	Inh: -3.0 % K _i : 30000.0 (nM)	Inh: 2.0 % K _i : 15576.9 (nM)
5 EX00000005		Inh: 55.0 % K _i : 8444.2 (nM)	Inh: 30.0 % K _i : 10370.4 (nM)	Inh: 74.0 % K _i : 2291.4 (nM)	Inh: 99.0 % K _i : 53.5 (nM)	Inh: 18.0 % K _i : 30000.0 (nM)	Inh: -24.0 % K _i : 15576.9 (nM)
6 EX00000006		Inh: -4.0 % K _i : 21428.6 (nM)	Inh: 6.0 % K _i : 13333.3 (nM)	Inh: -12.0 % K _i : 19565.2 (nM)	Inh: 1.0 % K _i : 15882.4 (nM)	Inh: 1.0 % K _i : 30000.0 (nM)	Inh: -2.0 % K _i : 15576.9 (nM)
7 EX00000007		Inh: 0.0 % K _i : 21428.6 (nM)	Inh: 7.0 % K _i : 13333.3 (nM)	Inh: -4.0 % K _i : 19565.2 (nM)	Inh: -10.0 % K _i : 15882.4 (nM)	Inh: -8.0 % K _i : 30000.0 (nM)	Inh: -7.0 % K _i : 15576.9 (nM)

Each row is a compound; each column an off-target receptor. ⊗ = Negative modulation; ⊕ = Positive modulation. The color of the circle indicates the relative likelihood of engagement with that receptor at the unbound plasma concentration (C_u) entered, based on the C_u/K_i of reference drugs with clinical data. Green = LOW likelihood; amber = MEDIUM likelihood; red = HIGH likelihood; grey = no plottable reference drugs exist.

To learn more about off-target risk profiles in D360, or the complete Secondary Intelligence application, contact will.redfern@certara.com

Learn more



About Certara

Certara accelerates medicines using proprietary biosimulation software, technology and services to transform traditional drug discovery and development. Its clients include more than 2,600 biopharmaceutical companies, academic institutions and regulatory agencies across 70 countries. Visit certara.com | Copyright ©2025 Certara. All rights reserved.