



# Deepening Digitalization in Drug Discovery at PTC Therapeutics

## Company Overview

PTC Therapeutics is a biopharmaceutical company based in New Jersey that focuses on the development and commercialization of innovative therapies for rare genetic diseases.

## Property Prediction in Support of Drug Discovery

The Medicinal Chemistry Team at PTC Therapeutics selected PhysChem Suite in the 2010s for its high accuracy and extensive compound coverage to calculate important physicochemical properties such as the acid dissociation constant ( $pK_a$ ), and the partition and distribution coefficients ( $\log P$  and  $\log D$ ) on which they base key decisions.

A decade later, the organization wanted to move away from the manual process of exporting their data into a separate spreadsheet, especially when needing to quickly compare structure-related property trends of multiple compounds. They shifted their focus towards digitalizing workflows and integrating tools and systems for expanded use and a better return on investment. As part of this, they wanted to investigate changes to their deployment of Percepta property predictors, to align with evolving organizational goals and needs.

With flexible deployment options of Percepta available, the Research Informatics team at PTC Therapeutics chose batch deployment of Percepta prediction modules which allows for high-throughput screening (HTS) of hundreds of thousands of compounds with minimal user intervention, providing the medicinal chemists with quick and seamless access to predicted data.

“ We’ve lowered the energy barrier to using the [Percepta] software by putting it right into the data aggregation system our chemists use every day. ”

– Christie Morrill



## Seamless Integration with the Dotmatics Platform

PTC Therapeutics were able to integrate Percepta Batch with their Dotmatics Notebook Informatics Platforms which enables immediate population of the relevant predicted  $\log P$ ,  $\log D$ , and  $pK_a$  values directly into their ELN and data aggregation systems. This gives their chemists instant access to the physicochemical properties in the systems they already use, significantly improving their workflow.



## On-Demand Data Access

The Dotmatics integrated deployment invokes Percepta Batch and writes data directly into PTC Therapeutics' existing database, ensuring a smooth workflow and minimal disruption. The updated access to property prediction values through the ELN gives the chemists more convenient, on demand access to all the relevant information for any compound in the company's portfolio.



## More Efficient Decision-Making for Compound Synthesis

With over 500,000 compounds in PTC Therapeutics' compound database, Percepta Batch makes data analysis significantly more efficient. The scientists use the predicted values from Percepta in conjunction with Certara's D360TM, a data visualization tool, to identify trends related to the physicochemical properties of their active compounds. Access to fast, reliable property values within the integrated system allows for rapid hypothesis testing and validation, accelerating the drug discovery process through informed decision making.



## Greater Data Integrity Through Collaboration

Previously, properties calculated by the Percepta desktop application were manually copied into an Excel sheet for analysis. These files were rarely shared amongst chemists, potentially resulting in duplication of work in what was already a time-consuming process. The Percepta Batch integration means that property calculations are automatically executed for any new compound entered into their ELN. The predicted property data is then available, company-wide, for easier access, effective collaboration, and informed decision-making.

“ We can now query the database table to see the compounds with a certain pattern of physicochemical properties. I feel this is the biggest benefit that we get out of this batch software. ”

– Prakash Balakrishnan

## Accelerated Drug Discovery Through Enhanced Digitalization

Integration of Percepta Batch has enabled PTC Therapeutics to move a step closer to digitalizing their drug discovery process. Medicinal chemists are now able to leverage critical property prediction data in informatics systems that are part of their daily workflow to select optimal candidates for investigation, optimize leads more effectively, and improve their understanding of the structure property relationships of their lead compounds, accelerating their innovation as a result.



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