

# Metabasis Therapeutics speeds time to market for important disease therapies with dynamic CADD technology running on a powerful IBM supercomputer.

## Overview

Metabasis Therapeutics, Inc. San Diego, CA, United States www.mbasis.com

# Industry

• Life Sciences

## **Products and services**

- IBM System p5 575 server
- IBM AIX V5.3 operating system



"Leveraging powerful IBM technology positions us to commercialize our unique solution, which will enhance and accelerate the drug-discovery process industrywide."

-Metabasis Therapeutics, Inc.

Metabasis Therapeutics, Inc. (Metabasis), is a biopharmaceutical company that discovers, develops and commercializes drugs used to treat metabolic and liver diseases. The company centers its research on developing treatments for some of the most common and widespread diseases.

# Challenge

Metabasis wanted to develop more accurate, easy-to-use computer-aided drug design (CADD) methods to accelerate the drug discovery process. The company developed accurate Free Energy Perturbation (FEP)-based CADD software, which improves the reliability of predictions on which drug design decisions are based—reducing the time it takes to find suitable drug candidates to evaluate in human clinical trials. But the company needed a high-performance computing environment for its FEP calculations.

# Solution

Teaming with IBM, Metabasis deployed an IBM System p5® 575 supercomputer running the IBM AIX® V5.3 operating system to enhance throughput for its CADD solution and to perform numerical computations. The supercomputer's 16 powerful processors can process certain stages of complex computations in parallel, further accelerating the drug discovery process. Metabasis has successfully used the CADD application running on the System p5 575 server to complete validation for ten structurally diverse sets of small organic molecules and for several inhibitors.

## **Benefits**

Metabasis's first-of-its-kind CADD solution significantly reduces drug-discovery time and costs by eliminating about 80 percent of the compounds to be synthesized and tested in the lab for a given drug target—enhancing the potential and speed of bringing the new drugs into the marketplace. With the solution, the company can facilitate better selections of candidate compounds to be synthesized and tested in the lab. Plus, Metabasis has positioned itself to commercialize the unique solution, which would enhance and accelerate the drug discovery process industrywide.



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