



## Modern Drug Design Discovery Enhanced by Parallel Computing

The College of Pharmacy at Western University of Health Sciences accelerates drug design discovery with powerful GPU solutions from Exxact Corporation.

### OUR CUSTOMER

Founded in 1977, Western University of Health Sciences has had a special mission: Educating tomorrow's health-care professionals with a combination of scientific excellence and a humanistic, compassionate approach to patient care.



The College of Pharmacy at Western University of Health Sciences is committed to providing a learner-centered academic and professional environment by offering its expertise in comprehensive drug therapy management. The areas of research include Pharmacology, Pharmaceutics, Pharmacokinetics, Drug Metabolism, Physiology, and Molecular Immunology.

## THE GOAL

The College of Pharmacy at Western University of Health Sciences utilizes computer simulation to explore the properties and functions of biomolecular systems. Through a combination of theory, experimentation, and simulation, Western-U conducts research and investigates the structural dynamics of complex biomolecules and how they affect physiological functions and diseases- in order to gain new perspectives in modern drug design and advanced therapeutic development.

In order to achieve this goal, Western-U relies on the AMBER molecular dynamics software package, which utilizes NVIDIA's advanced GPU computing power to accelerate the investigation of biomolecular models.

## THE CHALLENGE

As a new researcher, setting up a cluster that fulfills the unique computational requirements of AMBER can be overwhelming. AMBER requires a customized solution that can quickly process computational data on multiple compatible software platforms specialized for studying calcium binding proteins, membrane channels, G protein-coupled receptors, kinase proteins, and liposomes. Only high-performance systems customized with advanced parallel computing technology are capable of modeling cutting-edge, free-energy force field simulations.

## THE SOLUTION

When deciding the right solution to deploy for this project, Western-U turned to Exxact for technical expertise in GPU technology and familiarity with AMBER software systems to determine the ideal cluster configuration for performance optimization. In order to ensure a successful deployment, Exxact worked closely with Western-U and multiple software providers, including AMBER and Bright Cluster Manager, to fully understand the requirements for this specialized research. After doing extensive research on Western-U's precise performance requirements, Exxact's team of engineers developed multiple GPU platforms in order to benchmark performance, power efficiency, and cost. This led to the configuration of an ideal turnkey solution equipped with the latest NVIDIA Kepler-based GPU accelerators.

By maximizing simulation speed with parallel computing power from NVIDIA GPU accelerators, Exxact's GPU cluster empowers Western-U to tackle drug design workflow, test increasingly complex theories, simulate scenarios with greater levels of confidence, and minimize performance lag well into the future.

**"As a new investigator, Exxact helped design and customize our first GPU cluster that is a true turnkey solution, saving us lots of time from deploying, installing, and maintaining. We are impressed to see the simulation process accelerated by the GPU cluster. Exxact's expertise and wonderful support absolutely increase the ease of deployment for this project."**

*Lyna Luo, Assistant Professor of Pharmaceutical Sciences, College of Pharmacy, Western University of Health Sciences*

### About Exxact Corporation

Exxact is a leading provider of innovative high performance computing and visualization solutions, including servers, clusters, and workstations that are optimized for superior performance, efficiency, scalability, and precision. Each of our solutions is precisely built and meticulously tested for absolute customer satisfaction and product assurance. With our solutions, our customers are able to push the boundaries of research, optimize workflow, and accelerate the pace of research and discovery.

**Exxact Corporation | [www.exxactcorp.com](http://www.exxactcorp.com) | ISO 9001: 2008 Certified**

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