ComputaBio Has Launched Molecular Dynamics Simulation Services for Drug R&D Projects

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ComputaBio, a US supplier of professional computational biology services, has launched molecular dynamics simulation services for industrial and academic customers to expedite the process of drug design.

ComputaBio, a supplier of professional computational biology services based in the US, has launched molecular dynamics simulation services for industrial and academic clients to better their capability for drug design and expedite drug development programs.

With the continuous improvements in both computer power and algorithm design, a tide of computer-aided drug design is creeping up. Molecular dynamics (MD) simulations, as a powerful supplement to theoretical calculations and experimental methods as well as a useful technique to effectively understand macromolecular structure-to-function relationships, play an increasingly important role in data-driven drug discovery.

Molecular dynamics simulations are widely used for the structure-function studies of common-seen molecules such as proteins, peptides, enzymes, lipids, and etc. It has evolved into a mature technique frequently seen in the fields of chemistry, material science, biomedicine, and physics. The applications of the technique mainly focus on three main issues, i.e., allosteric regulation, docking, and structure refinement. Only by appropriate conduction of the technique could lead to accurate approximation of real molecules' behaviors.

ComputaBio is pleased to provide a set of molecular dynamics simulation services including protein molecular dynamics simulation service, peptide molecular dynamics simulation service, lipid molecular dynamics simulation service, enzyme molecular dynamics simulation service, membrane protein molecular dynamics simulation service, and replica exchange molecular dynamics (REMD). With a mature and reliable molecular simulation platform and powerful capacity in data analysis, ComputaBio is confident in satisfying its global clients and getting more and more credits from its services.

"The detection cycle takes only 3-5 days. It saves our clients' time." Says Gary Williams, Senior Scientist of ComputaBio, "We also provide the raw data and calculation result analysis, a solution to help our

clients improve effectiveness and cut the cost."

To better support scientists in drug development, ComputaBio also provides biological data analysis, drug design, molecular docking, protein sequence analysis, protein structure modeling, quantum chemistry, virtual screening, and other services. Visit the company's website (https://www.computabio.com/) for more information of the newly launched molecular dynamics simulation services and other services.

About ComputaBio:

Based in the US, ComputaBio is a supplier dedicated to providing professional computational services. The company has evolved into a customer-centered business and has a team of experienced scientists to ensure work quality. Except for services in molecular dynamics simulations, drug design, virtual screening, and quantum chemical calculations, the company also excels at the applications of various fields such as applications of biological data analysis, molecular docking, network analysis, protein structure modeling, and other essential process in drug discovery.