



# Accelerated VASP Pharmaceutical Molecular Model Computing with Intel® oneAPI Toolkits

Accelerating Medical  
Macromolecular Models on  
Volcano Engine with Intel®  
MPI Library and Intel® oneAPI  
Math Kernel Library

Medical macromolecular modeling plays a vital role in advancing the understanding of biological macromolecules, facilitating drug discovery and design, and guiding personalized medicine and vaccine development. However, these models are often computationally intensive due to their complexity and the duration of the modeling process. Intel® oneAPI Toolkits helped ByteDance improve the performance of these models for their customers. By using Intel® MPI Library and Intel® oneAPI Math Kernel Library, the solution improves performance by using highly optimized routines, leveraging HPC workloads to facilitate efficient communication between different nodes in a parallel computing system, thereby accelerating the applications and reducing R&D costs.

## Key Features



Biomedical  
Application



High-Performance  
Computing



Precision Medicine  
Analytics



Scalable  
Infrastructure

**Vertical:**  
Health & Life Sciences

**Country/Geo:**  
China/East Asia

**Use Cases:**

- Human Wellness Monitoring
- Precision Medicine Analytics

**Learn more:**

- [Intel Powers Volcano Engine to Accelerate VASP Pharmaceutical Molecular Modeling](#)
- [ByteDance Website](#)



*Volcano Engine provides customers with secure, reliable, high-performance, and easy-to-maintain enterprise-level cloud services. Intel® oneAPI Toolkits brings ByteDance another avenue to achieve better performance for HPC applications.”*

ByteDance Solution Architect in Beijing

## Intel Products and Technologies

- [Intel® Xeon® Scalable Processors Product Page](#)
- [Intel® oneAPI Toolkit Product Page](#)
- [Intel® MPI Library Product Page](#)
- [Intel® oneAPI Math Kernel Library Product Page](#)

