

Integrating artificial intelligence and machine learning VM allocation in the chemical industry using heterocyclic chemistry – A narrative mini-review

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ABSTRACT The chemical industry is rapidly transitioning toward cloud-enabled and high-performance computational infrastructures to support large-scale simulations, molecular modeling, reaction optimization, and data-intensive research. Efficient virtual machine (VM) allocation has become essential for improving throughput, scalability, cost-efficiency, and energy utilization for quantum chemical calculations, molecular docking, and virtual screening involving heterocyclic libraries. This narrative review examines the integration of artificial intelligence (AI) and machine learning (ML) techniques in VM allocation within chemical industry settings, with particular emphasis on heterocyclic compound research and computational chemistry applications. Drawing upon numerous documented applications of VM-based cloud deployment in chemical and materials science workflows, the review synthesizes current advances in AI-driven scheduling algorithms, predictive resource provisioning, reinforcement learning-based allocation models, intelligent load balancing, and adaptive auto-scaling strategies. It further discusses how ML-enhanced VM orchestration supports computational tasks in heterocyclic chemistry, including reaction pathway prediction, molecular property modeling, drug discovery simulations, and process optimization. Overall, integrating AI and ML with VM allocation represents a promising and scalable approach for advancing intelligent, efficient, and sustainable computational infrastructures within the modern chemical industry.

KEYWORDS Artificial intelligence, Machine learning, Virtual machines, Cloud computing, Resource allocation, Chemical industry, Heterocyclic compounds, Computational chemistry, High-performance computing, Predictive modeling.

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