CASE STUDY

CUTTING TIME TO INSIGHT: STREAMLINED PHARMACEUTICAL RESEARCH WITH SCALABLE HPC

Cambridge Crystallographic Data Centre fast-tracks its science with 400% faster AI model training

CUSTOMER

The Cambridge Crystallographic Data Centre (CCDC) is a global authority in structural science, curating the world's largest comprehensive database of small-molecule organic and metal-organic crystal structures. Based in Cambridge, UK, the CCDC plays a critical role in pharmaceutical research and development by enabling a deeper understanding of molecular interactions and behaviors. With a growing interest in applying AI to crystal engineering, the CCDC is using predictive models to identify coformers that could improve the performance of drug formulations.

CHALLENGE

The Cambridge Crystallographic Data Centre (CCDC) set out to answer a vital pharmaceutical question: Can AI predict which coformers are most likely to co-crystallize with a given drug?

The answer could improve how medicines are absorbed, stored, and delivered. But training AI models to make predictions requires enormous computing power—which is limited with the CCDC's local systems.

Key challenges included:

- Limited GPU power with in-house computing sources
- Incompatible scheduling with academic HPC resources
- Duration of model training—each test could take a month
- Trial-and-error tuning of AI models almost impossible to reach at scale

SOLUTION

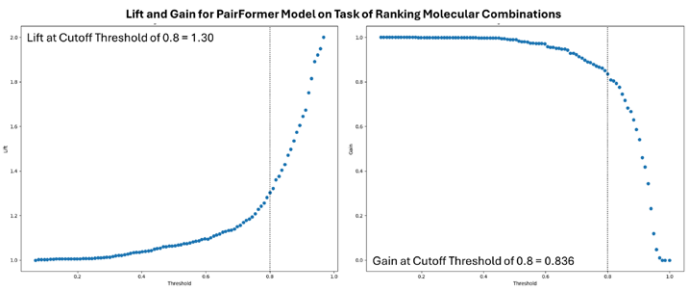
Partnering with Viridien gave the CCDC:

- Access to a powerful GPU infrastructure typically not accessible to research centers
- On-demand, scalable high-performance computing (HPC)
- Expert technical support to set up, manage, and optimize AI workflows

RESULTS

- **4x faster** model training (weeks instead of months)
- **Greater flexibility** to test more AI configurations
- **Confidence** in the final model's accuracy and performance
- **Dramatically shortened timelines** – the project could've been completed in 1/6th the time with Viridien's tailored HPC solutions from the start

By speeding up their AI research with Viridien's HPC Cloud capabilities, the CCDC has the capacity to help pharmaceutical companies design better drugs faster, bringing critical therapies to patients more efficiently.



Performance metrics for the CCDC model ranking an unordered list of molecular combinations. "Threshold" indicates potential cutoff scores for classifying a combination as positive or negative. "Lift" indicates improvement above random chance, while "gain" shows what percentage of the positives are captured. Both figures reveal how much the model will help in the prediction of coformers.

> "We were able to confirm that our model is the best model we could get —it wouldn't have been possible using our own architecture"
>
> **Jeff Lengyel, Research Scientist, Cambridge Crystallographic Data Centre**

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