

## **Exscalate4Cov performs the most complex supercomputing experiment to identify new therapies for COVID-19**

The Exscalate4CoV consortium, coordinated by Dompé farmaceutici, has conducted the biggest supercomputing experiment ever done on the SARS-CoV-2 virus in order to find potential drugs to treat COVID-19.



During the supercomputer-based experiment, more than 70 billion molecules have been tested on 15 active interaction sites of the virus by evaluating more than a thousand billion interactions in 60 hours. The aim of this research is to find new molecules that could be effective against the new coronavirus.

The researchers within Exscalate4CoV managed to do this impressive work by using simultaneously Eni's HPC5, the most powerful industrial supercomputer in the world, and CINECA's Marconi100, as well as the virtual screening software accelerated by the Politecnico di Milano and Cineca, and the Exscalate molecular library from Dompé farmaceutici. By bringing together all these technologies, the new goal of simulating 5 million molecules per second has been reached.

At the end of the first phase of the research, the generic osteoporosis medication, raloxifene was selected as the best possible existing drug that may reduce the symptoms of COVID-19. On 27 October 2020 the Italian Medicines Agency, AIFA authorised the phase three human clinical study of raloxifene as a potential treatment for patients who present few symptoms. The current goal of the project is to enrich the “molecular library” and find new potential molecules for an effective drug

cures COVID-19.

The results coming from the simulation will be shared within the scientific community on the open science MEDiate portal. This is the most comprehensive scientific source of knowledge on Sars Cov 2 virus available globally.

## More information

Exscalate4CoVpress release

Using European supercomputing, the coordinator of an EU-funded research project announces promising results for potential treatment

European supercomputers join pharmaceutical companies in hunt for coronavirus drug

Using European supercomputing to treat the coronavirus

## Related topics

HPC

Investing in network and technologies

---

### Source URL:

<https://digital-strategy.ec.europa.eu/news/exscalate4cov-performs-most-complex-supercomputing-experiment-identify-new-therapies-covid-19>