

THE EUROPEAN MOONSHOT FACTORY

MAJOR MILESTONE FOR THE JEDI COVID19 GRANDCHALLENGE THE FIRST EUROPEAN DARPA-TYPE CHALLENGE

- Stage 1 of the **JEDI Billion Molecules against Covid19 GrandChallenge** is completed. The challenge posed to each participating team was to screen a billion molecules on their interaction with Covid19 ('affinity')
- An estimated **54 Billion molecules were screened**, many of which are novel compounds - a key step forward at a time when repurposing of existing drugs (hydroxychloroquine, remdesivir..) is disappointing
- 10 Million hours of high-performance computing were used
- More than **130 teams from the best institutions and companies** in the world participated, representing 500 scientists
- This GrandChallenge is a radical new approach for pre-clinical **drug discovery** & a major step for **pandemic preparedness**
- The Scientific Committee is assessing results to determine if a team reached the target and wins the **250.000 Euro Prize**

-PRESS RELEASE-

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MAJOR MILESTONE, MASSIVE NUMBER OF MOLECULES SCANNED IN-SILICO

Stage 1 of the JEDI Billion Molecules against Covid19 GrandChallenge has run between May 4 and July 17. The past 10 weeks since the launch were an incredible success, with the participation of 130 teams. This represents around **500 scientists from the best private and public institutions of the world**, who worked intensively to fast-track the route to a therapeutic treatment against Covid19. Using extensive libraries of compounds, they screened an estimated 54 billion molecules to evaluate their blocking interaction with the SARS-CoV-2, for a total of more than 10 million hours of computing power mobilized.

André Loesekrug-Pietri, Director of the Joint European Disruptive Initiative, the European Darpa, highlights that *"the JEDI Billion Molecules Grand Challenge is one of the most ambitious attempts to radically accelerate the preclinical drug discovery process. In less than 5 weeks, JEDI has been able to mobilize a global response with over 100 teams, a world-class Scientific Committee, to identify the right challenge for maximal impact, and to work in close coordination with other major initiatives"*. He adds *"this is the **operational start of JEDI, the European agency for disruptive innovation**, with a major success and hopefully a significant contribution to science and global health"*.

DISRUPTING PRE-CLINICAL DRUG DISCOVERY

JEDI has high hopes for the results generated by the **new, innovative drug discovery approach** that was developed during the first stage of the Challenge.

Sir Peter Ratcliffe, Nobel Laureate 2019 in Medicine and member of the JEDI Covid19 Scientific Committee underlines *"The completely new method of drug discovery developed by JEDI during this GrandChallenge addresses problems extending far beyond the Covid19 crisis, potentially opening the door to a new way to tackle worldwide pandemics with an unprecedented efficiency."*

Indeed:

- The method developed by JEDI – targeting the process of generating hit compounds ready for clinical testing – is **significantly less time-consuming & cost effective** than the usual approach: it is estimated to reduce costs of identifying hit compounds from 20 million to 500.000 Euros, and to reduce the cycle time from around 1–2 years to a few months.
- It **increases chances of finding hit compounds** thanks to the screening of massive amounts of new molecules – at a time where repurposing efforts seem so far disappointing (HCO, azithromycin, lopinavir/ritonavir, remdesivir, ...) – and to the use of an innovative cross-correlation approach to improve accuracy of simulations. **Inspired by climate scientists but never used in drug discovery**, JEDI asked candidates to use different computational methods – from Molecular Dynamics, Deep Docking, to Machine Learning - to screen interactions between molecules and 6 pre-selected protein targets of the virus. After comparing results generated by these different approaches, participants had to build a list of 10.000 top-ranked compounds for at least 3 protein targets. **Prof. Thomas Hermans**, Program Manager of the JEDI Covid19 GrandChallenge points out that *“combined with additional cross-correlation analysis performed by the Scientific Committee during evaluation, this method has high chances to increase the hit rate at the end of the process”*.

A GLOBAL & COLLABORATIVE EFFORT

This success has been the fruit of an intensive collaboration between JEDI and other key actors involved in global efforts to fight the SARS-CoV-2, particularly with Folding@Home -whose director participates in JEDI’s Scientific Committee- as well as with the University of Texas initiative, and the Coronavirus Structural Task Force. The resources pulled by the GrandChallenge Strategic Partners include the AXA Research Fund - which was instrumental in launching this GrandChallenge - as well as Merck Group and the High Performance Computing consortia Genci and PRACE. **Prof. Adolfo Garcia-Sastre**, Director of the Global Health & Emerging Pathogens Institute at Mount Sinai and member of the Scientific Committee: *“This is a great initiative for the best scientific minds to come together to address an immediate need triggered by the current pandemic.”*

NEXT STEP, ASSESSING THE RESULTS & MOVING TO STAGE 2 : IN-VITRO VIRAL SUPPRESSION

Building on these lists, the JEDI Covid19 Scientific Committee will now move to create “ultimate lists of compounds”, from which the most promising molecules will be identified to be synthesized and experimentally tested in assays. Depending on their outcome, each candidate team will be attributed a “score”. To be considered for the 250.000 Euro prize, teams need to have included in their results at least one compound with a 100 nanomolar or better dissociation constant (“affinity”). **Prof. Charles Brooks**, Professor of Biophysics and Chemistry at the University of Michigan and member of the Scientific Committee: *“In reviewing Stage 1 contributions from the scientific community, I was extremely impressed with the innovation and scope of methods brought to bear in this extremely important drug discovery process.”*

Afterwards, Stage 2 of the GrandChallenge will **move forward from proven binding (Stage 1) to proven viral suppression** in a record time. It aims to obtain hard evidence of compounds that can lead to a 99% viral suppression at micromolar or lower concentration of the SARS-Cov-2 in cell assays. As a comparison, Remdesivir, currently considered as one of the most effective drugs against Covid19, has a 99% suppression at ~100 µM, which represents a performance at least 100 times inferior than the JEDI GrandChallenge. If successful, this stage would be a critical advance in the global efforts to find a therapeutic treatment against Covid19. **A true moonshot.**

About JEDI - the Joint European Disruptive Initiative (JEDI) is the initiative for disruptive innovation to bring Europe in a leadership position in breakthrough technologies. It is powered by 3.900 leaders of Europe’s deep tech ecosystem in 25 countries. JEDI is launching Tech GrandChallenges to push the frontiers of innovation, with a radical method based on excellence, no geographical return, speed, highest expectations & bold risk-taking. Driven by humanistic values, a purpose-driven approach to solve major societal issues in the environment, healthcare, digital, education, space & oceans through innovation. Europe needs a revolution to stay in the race, affirm its values, and lead.

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