ABOUT
S.A.F.A.N. BIOINFORMATICS is a small bioinformatic company based in Turin (Italy) with the mission of reducing costs and increasing efficiency of bringing new drugs to market.

Due to the high costs of the drug development process, within the pharmaceutical industry there is a general interest in applications that can be used for target deconvolution and off-target prediction such as the tool SAFAN-ISP, a new fragment based in-silico screening profiling technology.

CHALLENGE
New computational methods need a very accurate validation process in order to be accepted by the pharmaceutical companies.

Validation has been done on a limited number of cases in vitro or on a much larger amount of data in silico. The resulting statistical analysis was extremely important for SAFAN-ISP validation to promote its diffusion within the pharmaceutical industry.

HOW THEY USED EOSC SERVICES
SAFAN-ISP implemented a workflow running with a docker container performing a complete calculation within 15’ for each drug compound on one core.

With the support from EOSC DIH experts, the workflow was adapted to a cloud HPC environment to increase performance and make it able to analyse a dataset large enough for commercial purpose. Consequently, for pilot testing a subset of 10000 compounds were generated by analysing and comparing BindingDB data with ChEMBL.

Simulation runs were done in waves alternating between results analysis and refinement. Computational resources were used at CINECA. DICE provided support for porting of the code on the selected machine (Galileo100).

RESULTS
After executing SAFAN-ISP on the chosen compounds, an analysis of the affinities obtained was conducted.

IMPACT
The pilot resulted in an update of the TRL 4 to TRL 5, where SAFRAN technology is validated with an industrially-relevant dataset.