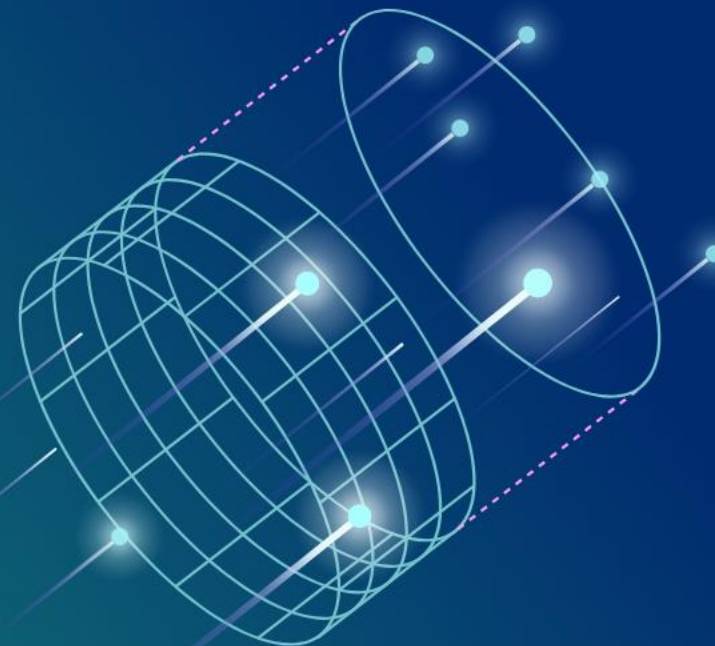


HEALTHCARE

# IMPROVING HEALTHCARE AND LIFE SCIENCES WITH HPC



ORGANISED BY:



IN COLLABORATION WITH:



UNDER THE AUSPICES OF:





# Carmine Talarico

DISCOVERY PLATFORM SENIOR SPECIALIST - Dompé  
farmaceutici S.p.A.

SCIENTIFIC RESPONSIBLE - Ligate

# IMPROVING HEALTHCARE AND LIFE SCIENCES WITH HPC

LIGATE

The game changer in drug discovery

November 21, 2022 - Prague CZECH REPUBLIC



LIGATEPROJECT.EU



# THE LIGATE PROJECT



# THE LIGATE PROJECT

## PROJECT FACT-SHEET

- LIGATE
  - Ligand Generator and portable drug discovery platform AT Exascale
- CALL: **H2020-JTI-EuroHPC-2019-1**
- 11 PARTNERS – 5 COUNTRIES
- BUDGET: € 5,938,656.25
- TIMELINE
  - **Start Date: 01 Jan 2021 (36 MONTHS)**
  - NOW: M22

## SCOPE

- **Create and validate a leading application solution for drug discovery in High Performance Computing (HPC) systems up to the exascale level**

# THE LIGATE PROJECT

## CONSORTIUM



# THE LIGATE PROJECT

## BACKGROUND

- The covid-19 pandemic demonstrates conclusively that a top priority for society, now and in the future, is to be able to respond quickly to diseases with effective treatments.

**But are we using all available resources in the most efficient manner?**

# THE LIGATE PROJECT

## PROJECT AMBITION

- No automated industrial software solutions are available for drug discovery, integrating:
  - geometrical scoring,
  - pharmacophoric scoring function,
  - molecular dynamic free energy estimation

**The central goal of LIGATE is to create and validate a leading application solution for drug discovery in High Performance Computing (HPC) systems up to the exascale level**



# THE LIGATE PROJECT

## WORKFLOW



1

DEVELOP A PORTABLE AND TUNABLE DRUG DISCOVERY PLATFORM READY FOR EXASCALE HPC SYSTEMS TO RESPOND PROMPTLY TO WORLDWIDE PANDEMIC CRISES.



2

VALIDATE THE CADD SOLUTION ON A NOVEL PROBLEM OF SOCIAL INTEREST.



3

VALIDATE THE TECHNOLOGIES INTRODUCED IN THE CADD SOLUTION.

# THE LIGATE PROJECT

## OBJECTIVES

**Provide the platform in the form of a highly scalable workflow**

**Code and Performance Portability on Heterogeneous Accelerators**

**Integrated automatic setup and execution of free energy calculations**

**Exploit state-of-the-art AI techniques to speedup the virtual screening**

**Exploit state-of-the-art Big Data technologies for HPC**

**The platform to be a full integrated industrial solution**



# Thank you!

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