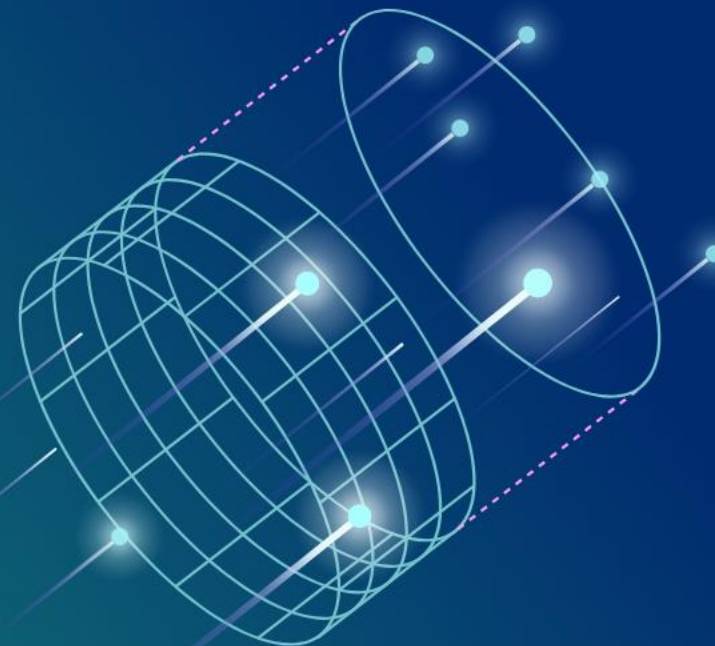


HEALTHCARE

# 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





# THE LIGATE AUTOMATED SOLUTION FOR COMPUTER ACCELERATED DRUG DISCOVERY USE CASE

# ASSESSING THE LIGATE APPROACH

## OBJECTIVES

A DEDICATED WORK PACKAGE WILL DEMONSTRATE AND ASSESS THE **LIGATE APPROACH** IN THE CONTEXT OF COMPUTER ACCELERATED DRUG DESIGN

USING AUTOMATED SOLUTION DEVELOPED BY THE PROJECT

DEPLOYMENT IN EUROHPC ARCHITECTURE HOSTED @  
CINECA AND IT4I

THE SOLUTION WILL BE TESTED AND VALIDATED

THE RESULTS WILL BE AVAILABLE  
FREE OF CHARGE

# ASSESSING THE LIGATE APPROACH

## EXECUTIVE SUMMARY

- VALIDATE PLATFORM ON KNOWN DATASETS
- VALIDATE INDUSTRIAL USE CASE

# VALIDATE PLATFORM ON KNOWN DATASETS

**GOLD STANDARD PROTEIN-LIGAND COMPLEX STRUCTURES COLLECTED FROM PDB AND PDDBind**

Gold-standard benchmark dataset

- Protein, Ligand, Pocket criteria
- ~7k pockets, 6k proteins, 1.5k ligands
- ~500 have binding affinity (PDDBind)
- Update with continuous PDB releasing

**GOAL:  
REACHING THE BEST  
CORRELATION WITH THE  
EXPERIMENTAL RESULTS**

# VALIDATE INDUSTRIAL USE CASE

## APPLICATION OF LIGATE WORKFLOW TO IDENTIFY ANTIVIRAL COMPOUNDS AND EXPERIMENTAL ASSESMENT

- Selection of Main Viral Enzymes from different viral species
- 3D structures modelling and selection of a subset of representative ones for *in silico* evaluation
- Collecting expression constructs for representative proteins enabling the Experimental validation (*Biochemical Assays and Xray/Cryo-EM experiments*)
- Running LIGATE pipeline to select the best chemical probes to be experimentally validated

**GOAL:  
IDENTIFICATION OF NEW  
COMPOUNDS BLOCKING  
VIRAL ENZYMES**



# SUMMARY

1. ASSESSMENT OF THE INTEGRATED PIPELINE ON GOLD STANDARD PROTEIN-LIGAND COMPLEX STRUCTURES
2. DEPLOYMENT OF THE LIGATE WORKFLOW IN AN INDUSTRIAL USE CASE TO IDENTIFY ANTIVIRAL COMPOUNDS
3. EXPERIMENTAL VALIDATION OF THE *IN SILICO* HYPOTHESIS ON DEFINED VIRAL ENZYMES

# Thank you!



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