IHI Call Days | Call 9

Accelerating ligand identification discovery for protein targets using novel datasets and ML methodologies

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Link to the IHI brokerage platform: https://ihicalldays2024.converve.io/

Challenges and objectives

Challenges:

- To accelerate the identification of the best starting points for future therapeutics through a systematic study of small molecules and the human proteome.
- To reduce time, failure rates and high costs associated with novel drug discovery.
- To address barriers to cross-sectoral collaboration between diverse disciplines to enable rapid scientific and technical innovations in life sciences.

IHI Specific Objectives (SO):

- SO2: Pre-competitive work that integrates fragmented health research and innovation efforts, bringing together health industry sectors and other stakeholders. Focusing on unmet public health needs, enable the development of tools, data, platforms, technologies and processes for improved prediction, prevention, interception, diagnosis, treatment and management of diseases, meeting the needs of end-users.

Public Health Need Addressed:

- ID of innovative methods to transform drug discovery for unmet public health needs

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Approach to solve the problem

This proposal aims to:

- Conduct the largest ever ligandability assessment of the human proteome and create a first in class data set of sufficient size and quality to train machine learning methods for predictive hit identification/expansion.
- Galvanise collaboration among a vast network of scientists & researchers from academia and industry, combining expertise across computational drug discovery, AI/ML, structural biology, medicinal chemistry, algorithm design, screening and assay development.

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Why this project is suitable for IHI

- A unique and large dataset of this type can only be created through a Public Private Partnership, with collaboration that requires cross-discipline and cross-sector expertise
- This proposal requires contributions from academics, large & small pharmaceuticals, biotech and tech SMEs bringing:

- Colleague expertise and experience
- Assays, screening technology, screening set design and implementation
- ML algorithm development. Data analytics, storage and handling.
- Sourcing thousands of proteins, small molecule libraries, large-scale data generation
- Wet-lab services

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Anticipated outcomes and impact

Outcomes

- A consistent, large dataset that enables ML algorithm development to underpin a new generation of 'predictive' drug discovery
- Identify proteins with high ligandability that initiates therapeutics research

Impact

- Following open science principles; accelerate target understanding and accelerate drug discovery, leading to future breakthroughs for treatments.
  - Empower the critical mass of science and people required that no single organization could bring
  - Reduce the duplication of effort often inherent in drug discovery approaches
  - Provide publicly available resources, knowledge and data that improve scientific reproducibility and research quality in drug discovery

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Expertise and resources needed

- We have:
  - Public partners to make proteins, undertake screening, manage the project
  - Industry partners bringing expertise, screening and proteins

- We are looking for:
  - Expertise in ML computational modelling for drug discovery
  - High throughput screening capability (DEL/ASMS)
  - Sources of protein reagents and biophysical assays

Expected Project Budget: €60M over 5 years

- €30M in-kind contributions via IKOP, IKAA and FC
- €30M matched funding from IHI

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IKOP: in-kind contributions to operational activities, IKAA: in-kind contribution to additional activities, FC: financial contributions