Covid19 Drug Discovery Workflow Platform (CDD-WP)

Cloud Enabled AI Driven Workflows for Drug Discovery and Design

Context

- ✓Our **CDD-WP has been tested on 60% of the drug discovery work streams**; built on KNIME workflows with Python scripts running on MS Azure Cloud. We want to test the scale and execution speed of these workflows on an **HPC platform**

- ✓We intend to use multiple of AI/ML frameworks on identified molecules/compounds/protein structures to **increase the reliability and trust from these AI results**

- ✓Our objective is to **deploy and test to run CDD-WP as a service and leverage multiple AI/ML frameworks** on possible Covid19 structures/compounds to aid in drug design/discovery process

Credits from Existing Works

* Computer Aided Drug Design/Discovery

TeachOpen CADD

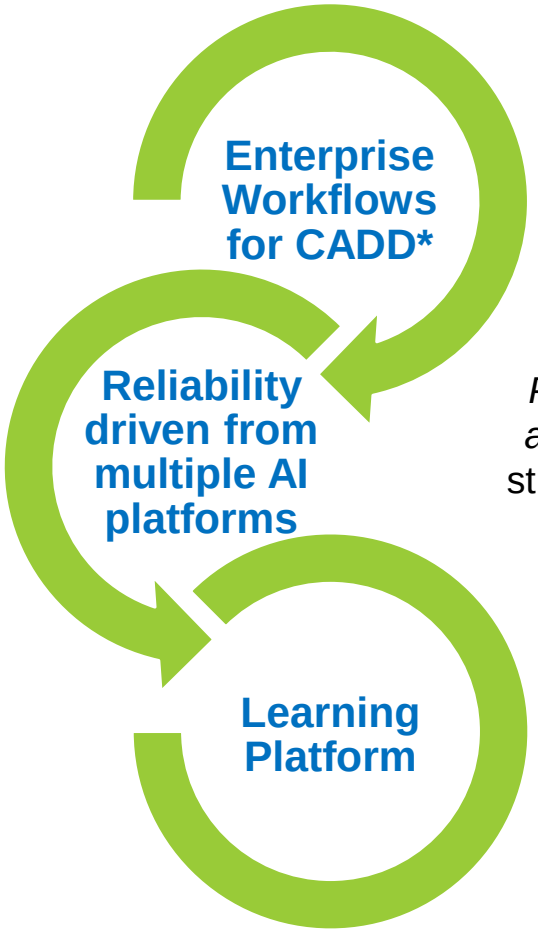
10+ generic workflows that are built for computer-aided drug design (CADD*) using KNIME that needs enterprise customization for Covid19

Google AlphaFold

5+ Covid19 Structure Predictions e.g. M_protein, Protein_3a, Nsp2, Nsp4, Nsp6 and PL-PRO C terminal

TCS

30+ compounds inhibiting the 3CL protease (3CL is essential for SARS-CoV-2's survival and replication in the host)

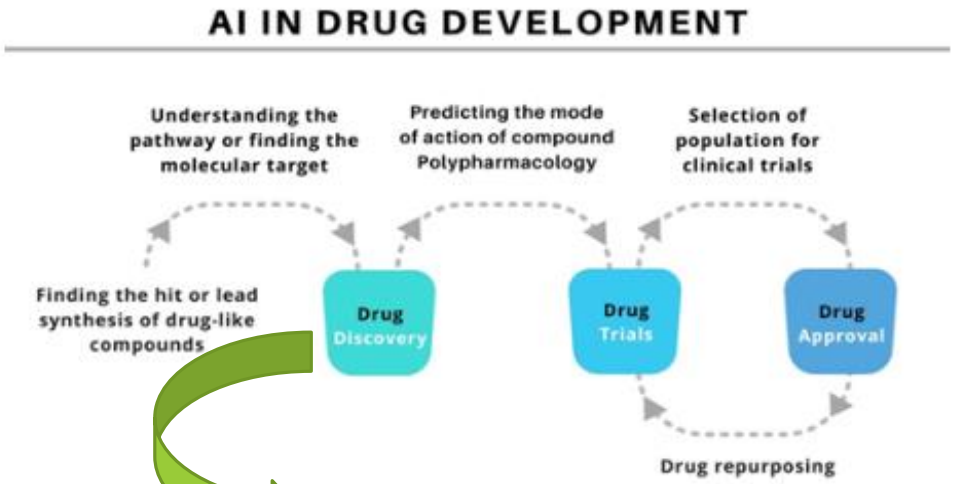


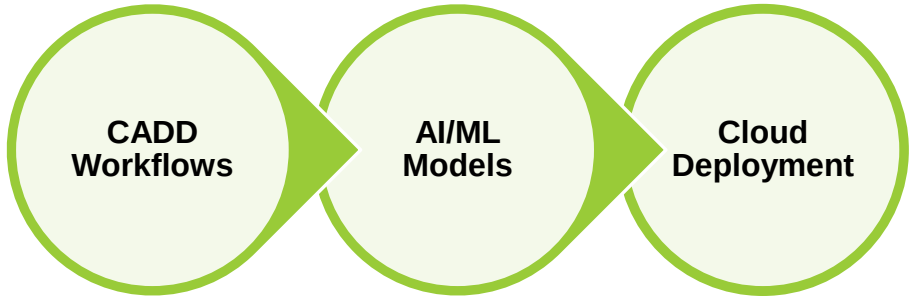
Ability to set up quick enterprise workflows for CADD* process

Platform should leverage already predicted protein structures from AI platforms like Google's AlphaFold

Scale the platform into a learning system to reduce biasness from identified compounds from multiple research studies

CDD-WP's Readiness

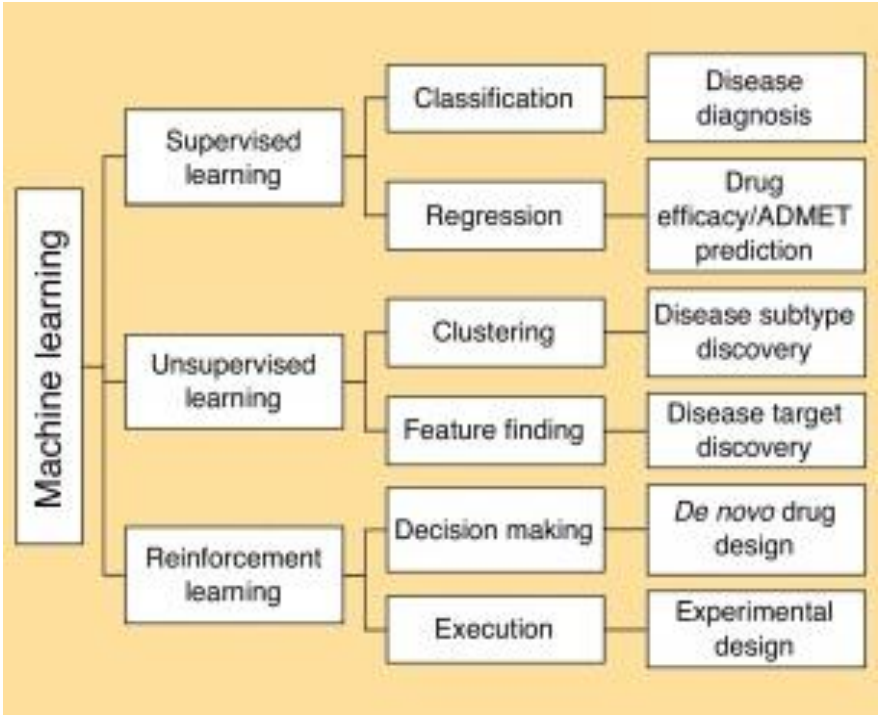




Run Drug Discovery as a Service

Sl No.	Steps	Digital Workflow ID	Workflow Available?	Python Scripts Available?	AI/ML Models Available?	Leveraging Existing Works?	Cloud Deployment Ready?
1	Compound data acquisition	CADD_W1	Y	Y	WIP	Y	Y
2	Molecular filtering: ADME and lead-likeness criteria	CADD_W2	Y	Y	Y	Y	Y
3	Molecular filtering: Unwanted substructures	CADD_W3	Y	Y	WIP	Y	Y
4	Ligand-based screening: Compound similarity	CADD_W4	Y	Y	Y	Y	Y
5	Compound clustering	CADD_W5	Y	Y	Y	N/A	Y
6	Maximum common substructures	CADD_W6	Y	Y	WIP	N/A	Y
7	Ligand-based screening	CADD_W7	Y	Y	Y	N/A	Y
8	Protein data acquisition	CADD_W8	Y	Y	WIP	Y	Y
9	Ligand-based pharmacophores	CADD_W9	WIP	Y	Y	N/A	WIP
10	Binding site similarity	CADD_W10	WIP	Y	Y	N/A	WIP
11	Structure-based CADD using online APIs/servers	CADD_W11	WIP	Y	Y	Y	WIP
11.1	Querying KLIFS & PubChem for potential kinase inhibitors	CADD_W12	WIP	Y	WIP	Y	WIP
11.2	Docking the candidates against the target	CADD_W13	WIP	Y	Y	Y	WIP
11.3	Visualizing the results and comparing against known data	CADD_W14	N/A	Y	N/A	N/A	WIP

CDD-WP's AI Models

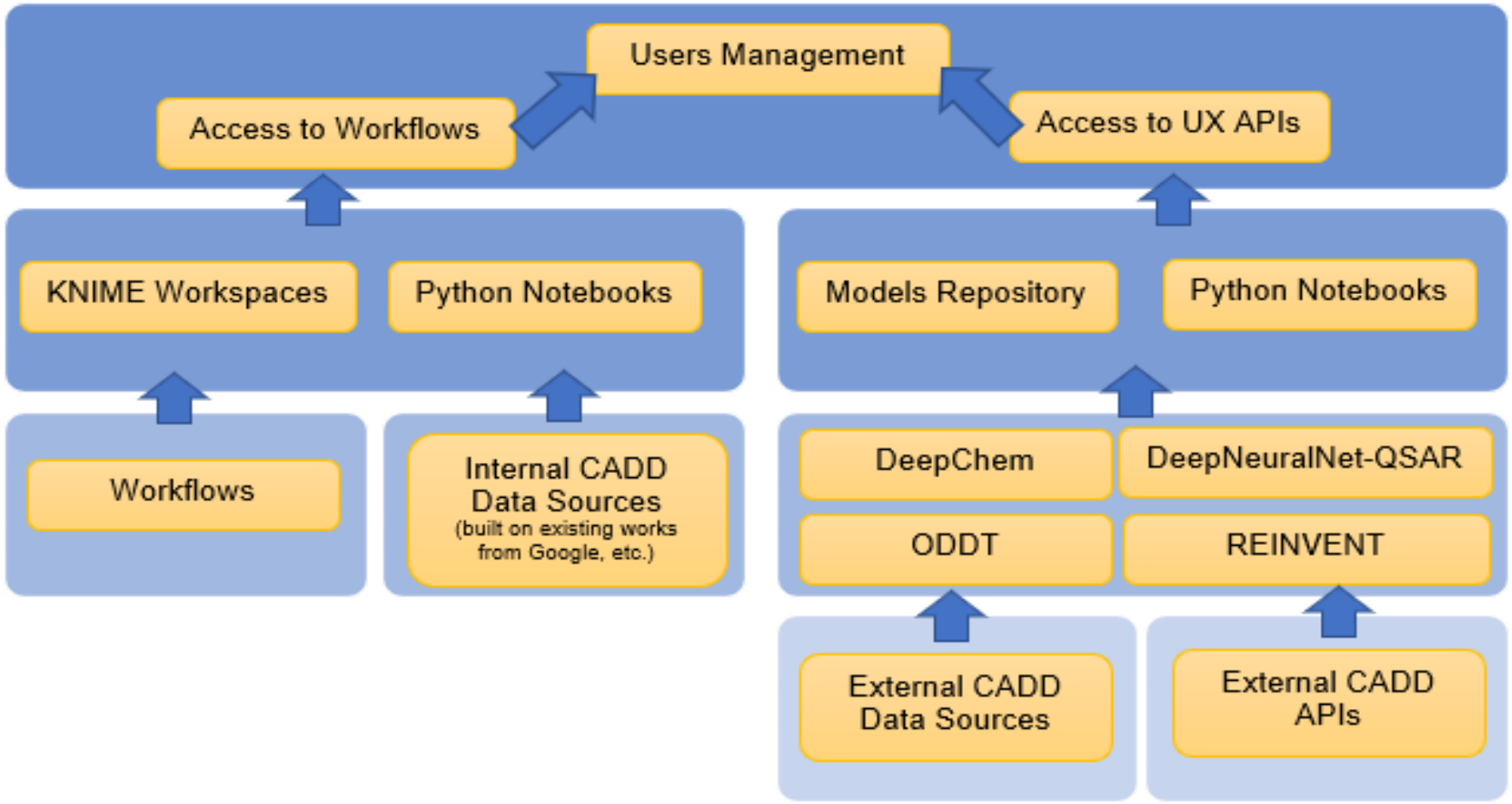


Drug Discovery Process	Drug Design Sub-Process	Applicable AI Models	Leverage Existing Works
Target Idenitification and Study	Prediction of Protein Folding	CNN	Google's AlphaFold
	Prediction of PPIs	FD/DCA	Google's AlphaFold
Hit Discovery	Drug Repurposing	Network Analysis	TCS
	Virtual Screening	SVM, AAE	TCS
	Activity Scoring	SVM, RF, CNN	TCS
Hit to Lead	QSAR	DNN	DeepNeuralNet-QSAR
	De Novo Drug Design	AAE, VAE	REINVENT, DeepChem
Lead Optimization	Evaluation of ADME/T properties	CNN	DeepChem, Open Drug Discovery Toolkit

We will be leveraging the below mentioned AI platforms and data sources in addition to ChEMBL/PubChem/PDB –

a) DeepChem
b) Open Drug Discovery Toolkit (ODDT)
c) REINVENT
d) DeepNeuralNet-QSAR
e) Google's AlphaFold (for 5 predicted protein structures)
f) TCS AI Virtual Screening (for 31 compounds)

CDD-WP's Functional Stack



CDD-WP's Benefits

* Computer Aided Drug Design/Discovery

1

Plug-in to any CADD* Process

Integrated CADD Workflows with base codebase available for implementation

2

Integrates with 3+ CADD AI Platforms

Deploy multiple AI/ML frameworks/models during an implementation cycle to improve the reliability score

3

CADD Workflows as a Service

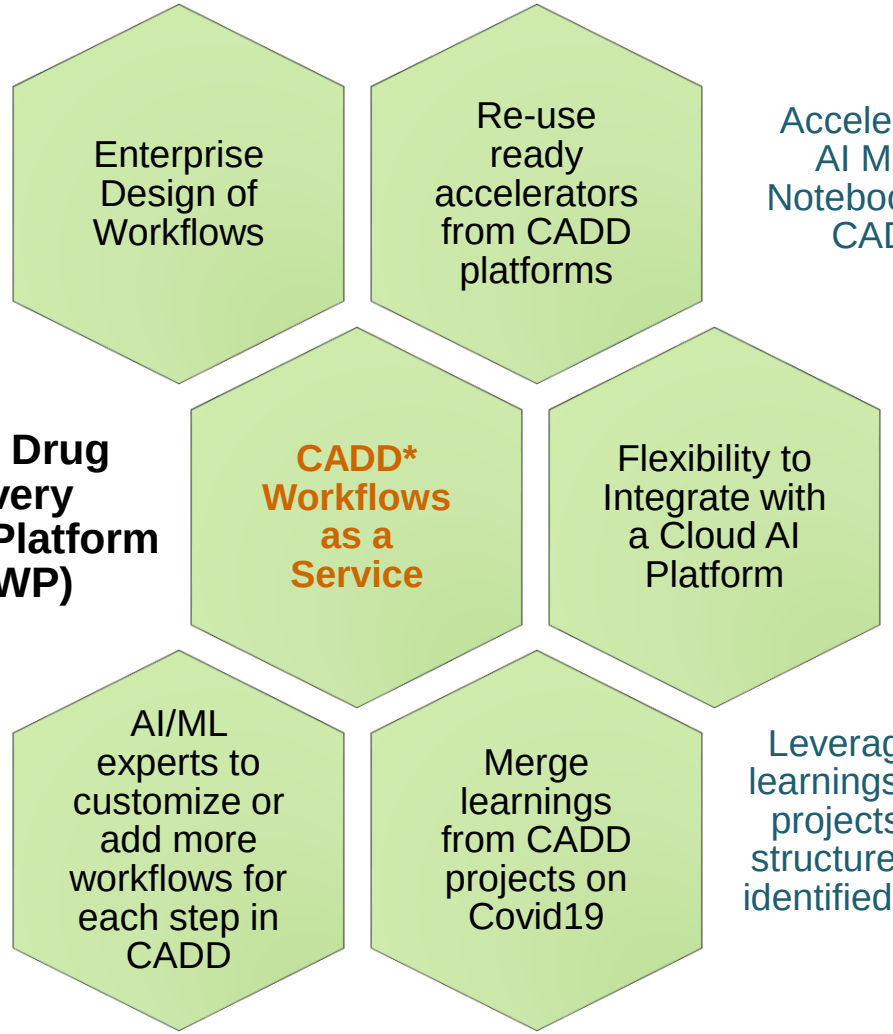
Data Management as a Service on identified compounds/molecules/ structures

- ✓ Helps to deliver the **Proof of Concept (POC) in 2-3 weeks**
- ✓ Easily scales up for enterprise adoption by using the **industry best practices in CADD as an integrated workflow platform**
- ✓ Improves reliability by leveraging **multiple CADD AI Platforms**

CDD-WP's Enterprise Scale

* Computer Aided Drug Design/Discovery

Workflows can be easily configured as per the CADD process for any research organization



Accelerators in form of AI Models, Python Notebooks from existing CADD platforms

CDD-WP can be easily extended and integrated with MS Azure AI/ML Platform

AI/ML experts to engage who have worked with cloud data lakes and enterprise workflow models

Leverage available learnings from CADD projects on protein structure predictions, identified compounds, etc.

Thank You

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