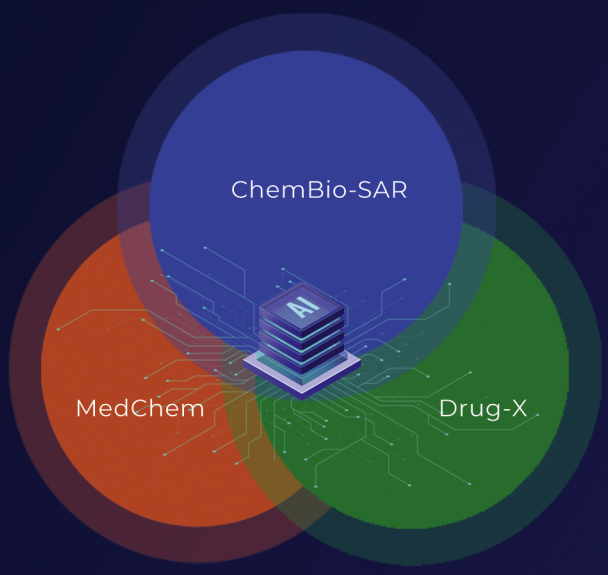
IMMUNOCURE® DISCOVERY SOLUTIONS

A pre-clinical small molecule drug discovery CRO integrated with chemistry facility leveraging AI & computational platform – AxDrug®

CASE STUDIES

- AxDrug® applied for 30 different targets with 100% success rate in discovering drug candidates
- Identified first in class molecules for the most intricate targets
- Successfully innovated best-in-class molecules with poly-pharmacology
- Modeled 3D structure and generated drug candidates for highly disordered proteins
- POC established for each program by synthesizing ~ 200 molecules



axdrug®

A FEW OF OUR CLIENTS

PennState College of Medicine · TUSKEGEE UNIVERSITY · tgen part of City of Hope · STINGRAY THERAPEUTICS

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IMMUNOCURE® DISCOVERY SOLUTIONS

HIGHLIGHTS

- Accurate protein structure prediction for complicated and orphan targets
- Identifying the cryptic pocket and druggability analysis
- AI generated large proprietary drug-like database
- Flexible framework applicable to any target
- Automated multi-parameter optimization with integrated AI and computational techniques

ADVANTAGES

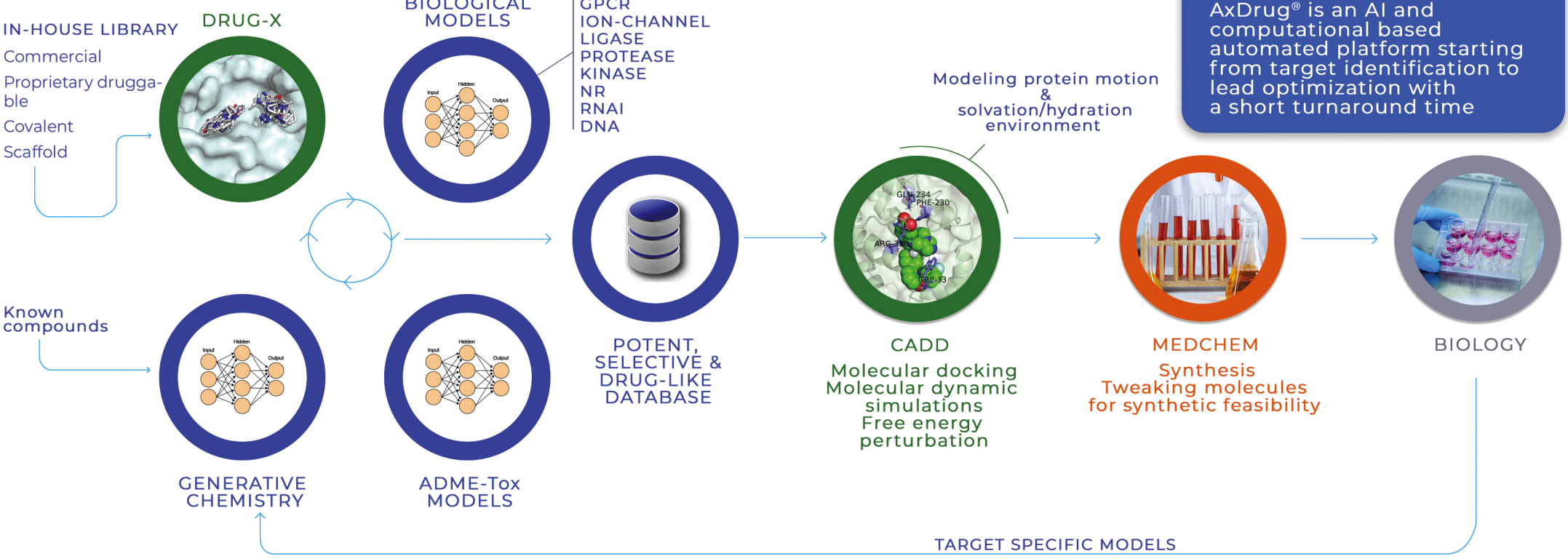
- Integrated AI and CADD platform to generate drug candidates with less turnaround time
- Generates quick hypothesis with validation
- Rapid virtual screening AI protocols
- Coordination of in-house AI, MedChem and Synthetic teams convert the virtual compounds into reality reduces cost and time
- Accurate prediction of efficacy, selectivity, and safety

IN-HOUSE SYNTHESIS FACILITY

IMMUNOCURE® DISCOVERY SOLUTIONS

axdrug® – AN INNOVATIVE AI DRUG DISCOVERY ENGINE

AxDrug® is an AI and computational based automated platform starting from target identification to lead optimization with a short turnaround time



ChemBio-SAR

- Generative Chemistry (GC) – Generation of potent, selective and drug-like compounds with graph-based transformers in a Reinforcement Learning framework
- *In vivo* and *in vitro* ADME-Tox models to reinforce the transformers in GC
- Empowering the discovery by GC and ADME-Tox models driven proprietary database
- Unlocking new possibilities with an advanced biological models for selectivity and polypharmacology
- Combining the AI models with computational chemistry to create a new era in drug discovery

Drug-X

- Recurrent Geometric Network (RGN) for end-to-end modeling of orphan proteins
- Unlocking the proteins by identifying the druggable pockets with mixed solvent sampling, and evolutionary methods
- Fragment-based scanning and geometry-based fingerprint generation for high-speed virtual screening of large databases
- Discovery of high-affinity molecules for difficult targets utilizing GC & Molecular Dynamic Simulations (MDS)
- Docking, MDS, water thermodynamics and FEP for prioritizing the desired compounds

MedChem

- Improving the desired properties and synthetic feasibility of the selected molecules
- Synthetic route estimation using big data
- Reaction mechanism estimation for solving complex bottlenecks with better yields
- Bioisostere replacement for improving the druggable properties
- Impurity predictions for better understanding of the synthetic protocols