XtalPi

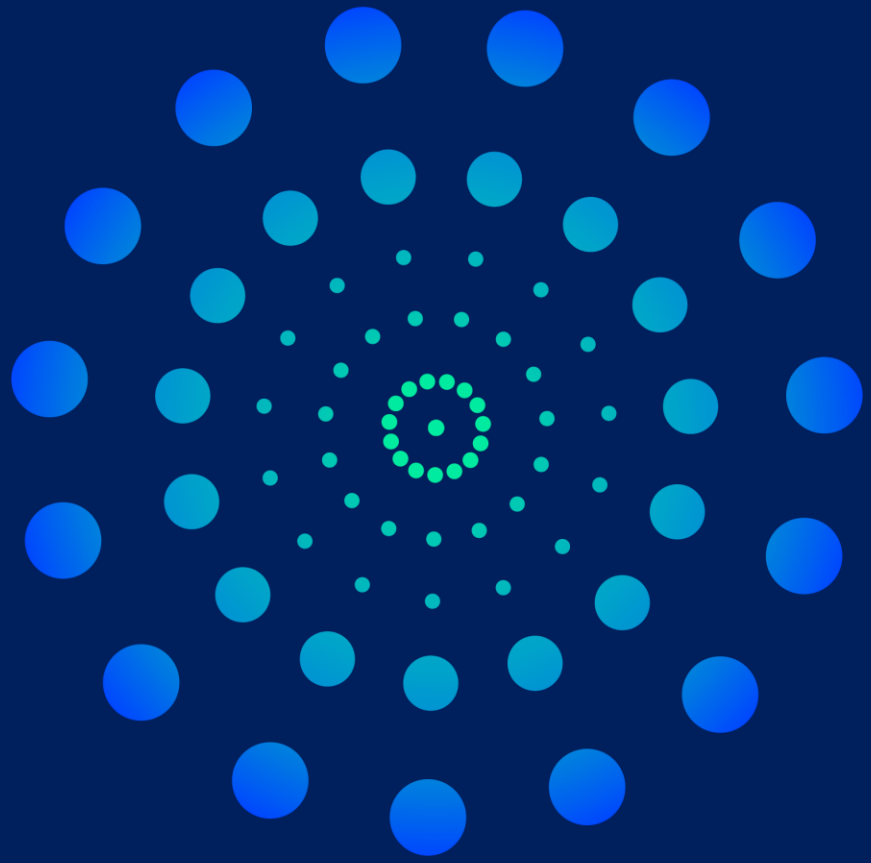
Accelerating Discovery with AI and Next-Generation Automation

XtalPi Corporate Introduction • Q1 2024

XtalPi

Content

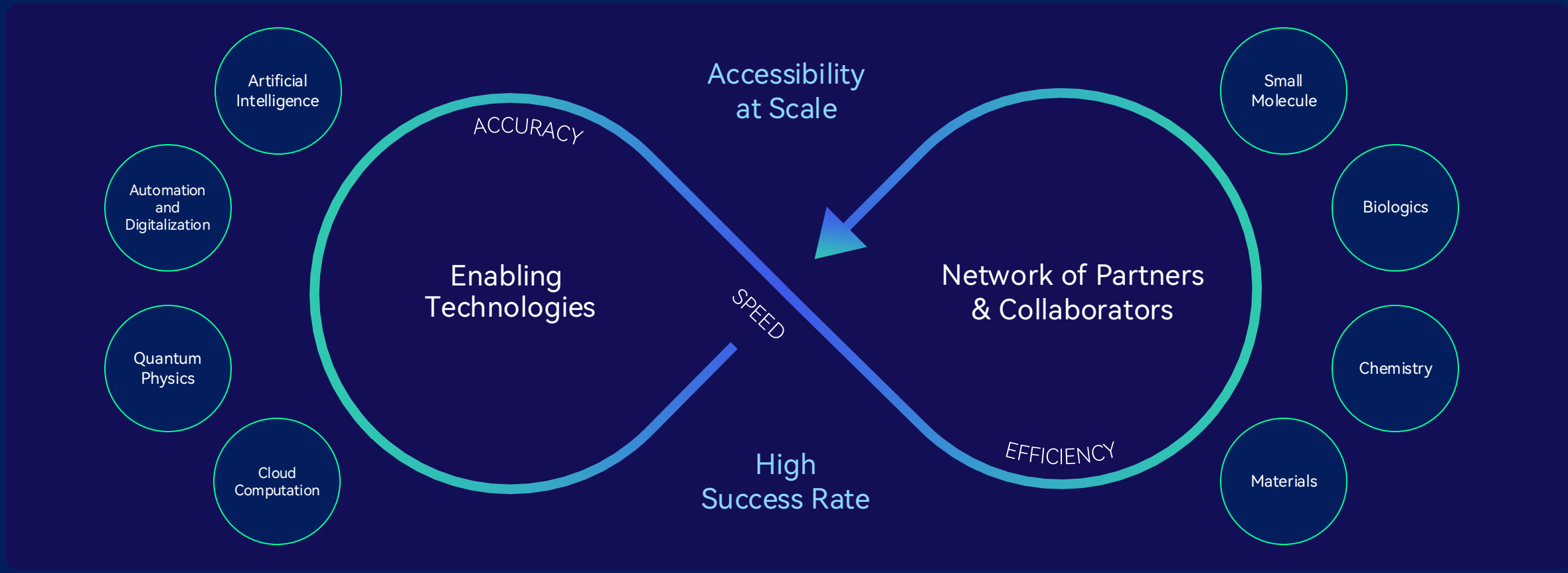
About XtalPi



PART ONE

We are a technology ecosystem company

We focus on creating accessible, enabling technologies at scale. We Provide partners of all sizes in molecular R&D with the foundational tools to accelerate the discovery of impactful, life-changing therapeutics and products.



Locations and Team

Our technical and management teams operate closely together across 4 different sites

120+
GRANTED PATENTS

70%
SCIENTISTS & TECH

10,000 + m2
LAB SPACE

700+
EMPLOYEES

Access our innovative technology ecosystem through various collaboration methods

Services & Solutions

- Traditional FTE or FFS model for discovery and development projects
- Access to our products and digital/computational platforms with a fee

Partnership

Leverage expertise and technological capabilities from both parties to co-develop or discovery different assets

Industry-leading, empowering drug discovery and development platforms

Small-Molecule Drug Discovery Platform and Solutions

- Integrated drug discovery services
- ID4Idea™: AI-based platform
- IDA4Gibbs™: High-accuracy computational chemistry platform
- Special Chemistry: ADC, PROTAC, DEL, peptides

Solid-State R&D Platform Driven by Automation + Computing

- Rapid, high-precision solid form screening and selection platform
- XtalCSP™: Crystal structure prediction platform
- MicroED: Structural analysis polymorph, salt, cocrystal screening
- AI-Driven, Automation-aided crystallization and execution

Intelligent, AI-Empowered Automation Technology Platform

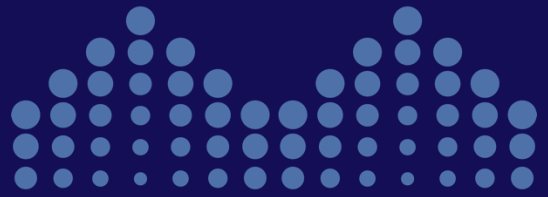
- Flexible, integrated automation for chemical and analytical processes
- Complete digitization software suite empowered by AI

Ailux Biologics

AI-Empowered Antibody Discovery and Engineering Platform

- XtalFold™: Complex structure prediction
- XenProT: The GPT for proteins
- Xentient: Predictive AI Suite
- Next-gen Engineering: New lead-opt options
- Raise the Bar: Elevating conventional campaigns
- Hard Targets: Challenging hit-gens

Discovery Platform that Drives Real Success



One step ahead of industry trends through integrating AI and automation with molecular R&D

XtalPi Journey

2015
Crystal Structure Prediction Platform
- XtalPi officially incorporated
- Released CSP platform

2018
AI-Powered Small Molecule Drug Discovery
- Established small molecule discovery platform
- Harnesses the power of AI for accurate discoveries

2019
Synergy between AI, R&D, and Researchers
- Established drug discovery labs
- Integrated services with AI, automation labs, and researchers

2022
Small Molecule and Antibody Discovery Platforms Commercialized
- Strong commercialization growth in small molecule and antibody discovery platforms

2023
LLM for Chemistry and Antibody Discovery
- Reshaping the new paradigm of biopharmaceutical and material research and development

Industry Developments

~90's - 2014
- Rapid breakthroughs in computer technologies
- Emergence of CADD
- Early HTS technology

2014 ~ 2018
- Development of AI technologies and cloud computing
- Improvements in accuracy of algorithms and computing infrastructure
- AI pharmaceutical industry slowly emerging

2018 ~ 2023
- AIDD commercialization on the rise
- Diverse array of business models emerging
- Strong AI pipeline developments,
- A small portion of companies beginning to transition towards platform-based business models

2023 ~ 2028
- Introduction of automation to the process has significantly improved quality and quantity of data volume
- Large language models revolutionizing the speed of vertical learning

Strong track record in partnering with major global pharma

2018
10-year collaboration initiated (Pfizer)

Pfizer

2022
COVID drug, Paxlovid, crystal structure solved in 6 weeks (Pfizer, 2022)

janssen Pfizer

2023
$250M USD drug discovery agreement (Lilly, 2023)

Lilly MERCK

2024
+ Our Future

> The collaboration with XtalPi is already changing the way Pfizer performs its screening work and has the potential to disrupt the industry as a whole."
>
> GEOFF WOOD
> PRINCIPAL SCIENTIST, PFIZER

> Our collaboration with XtalPi is transforming pharmaceutical development. By seamlessly incorporating computer simulations with our experimental formulation expertise in a "digital-first" approach, we are boosting drug development processes and positively impacting patients' lives."
>
> DR. JAN GERIT BRANDENBURG
> HEAD OF DIGITAL CHEMISTRY, MERCK KGAA

XtalPi

Small Molecule Drug Discovery

PART TWO

AI-driven platform to accelerate drug discovery phase transitioning

Proprietary technologies for de novo design, accurate predictions, and rapid synthesis to tackle challenging targets

Hit Discovery → Hit Identification → Hit-to-Lead → Lead Op → PCC

ID4Inno™

De Novo Compound Design

- Structure-based design
- Ligand-based design
- Virtual screening/HTS

Computational Chemistry

- Synthesizability assessment
- Physicochem. prediction
- Library enumeration

Automated Synthesis

Automation-aided Discovery Chemistry

- Singletons synthesis
- Scaffold synthesis
- Building block synthesis

High-throughput Experimentation

- Fixed/custom libraries
- Reaction optimization
- Automated analysis

Data Analysis

Med. Chem. Insights

- SAR analysis
- ADME assessment
- Toxicity evaluation

Chemist-centric ELN

- Reaction conditions
- Compound characterization
- Chemical sourcing

Biology Platform

Structural Biology

- Protein expression
- Cryo-EM

In-vitro Biology

- Biochemical assays
- Cell-based assays
- ADMET

In-vivo Pharmacology

- Disease models
- DMPK
- PK/PD

AI-driven novel compound design

Challenging targets are our primary focus

Automation-empowered chemistry scouting and synthesis

End-to-end data management & drug discovery solutions

Discovery platform that drives real success

SUPERIOR NOVELTY & DIVERSITY

90%

Success Hit/Lead Discovery Rate

- Molecular design and generation with screening technologies
- High-accuracy Computation
- Generative AI
- Predictive AI

HITS FOR CHALLENGING TARGETS

30+

Active Discovery Programs

Workflow designed to maximize the chance of finding good hits/leads that are difficult to come by for challenging targets

TEST FAST, SUCCEED (OR FAIL) FAST

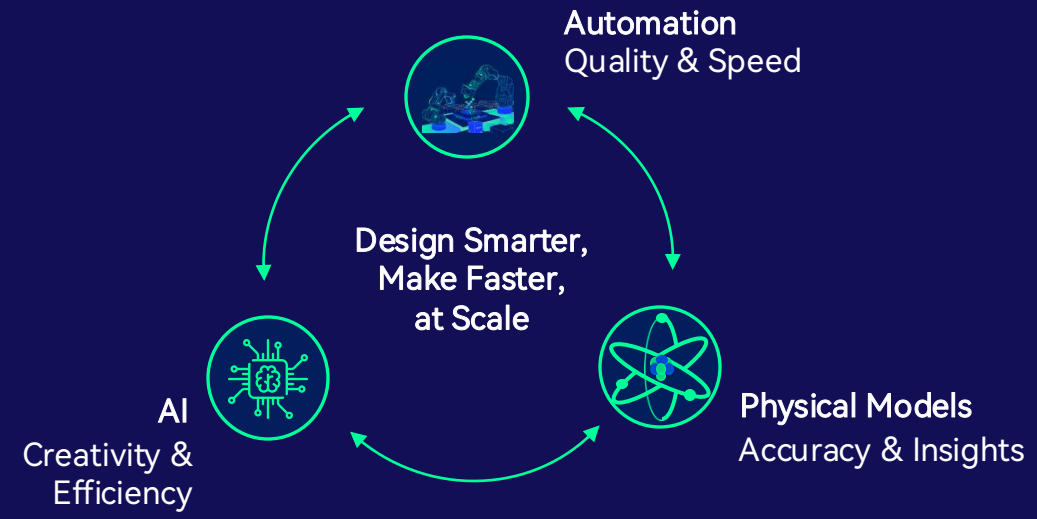
Up to 50%

Active Discovery Programs

Automated chemistry to accelerate the synthesis and testing of compounds to rapidly test hypothesis and generate valuable medicinal chemistry insights

Deploy proprietary AI & automation for early drug discovery

Target Structure Elucidation → **Hits Discovery** → HIT-TO-LEAD → **Lead Identification** → Lead Optimization

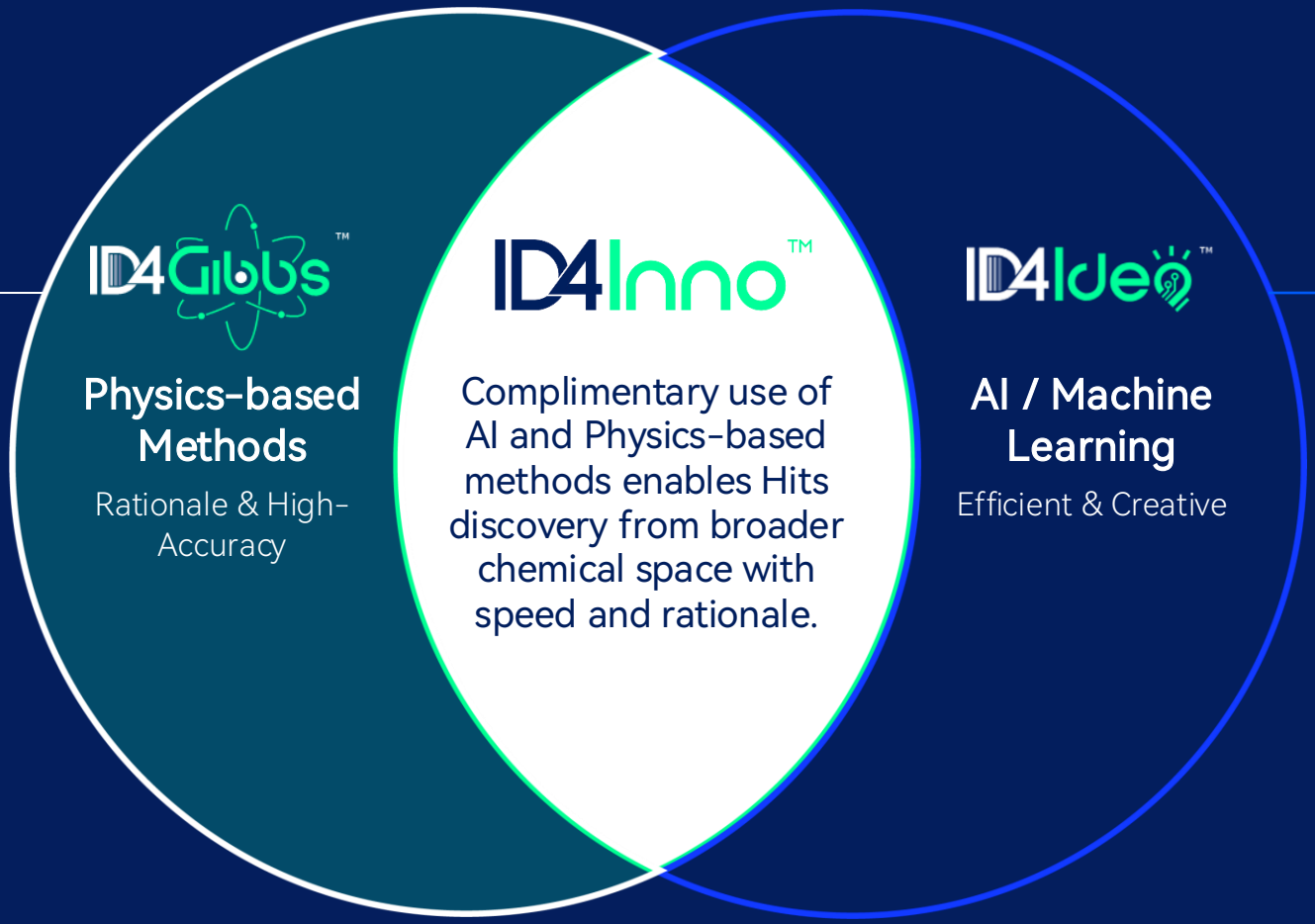


- Enable **best solutions** to discover novel Hits/Leads for challenging targets
- Deliver library compounds with speed, diversity, and throughput

ID4Inno: A proprietary platform combining AI efficiency with physics accuracy

Enhancing drug discovery with AI and computational chemistry to generate fewer, better compounds

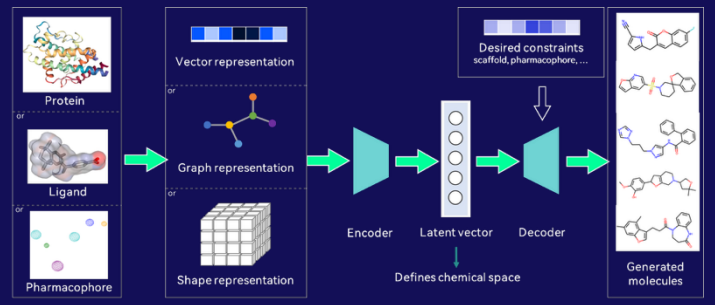
- First principle, no training required
- Extrapolate to new chemical space
- Accurate prediction
- Structural insights

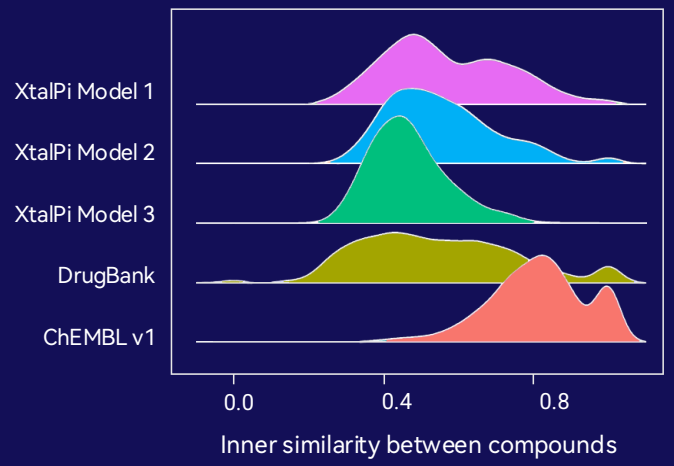


- Accurate, if similar to training set
- Generate novel ideas
- Computationally fast
- Handle large datasets

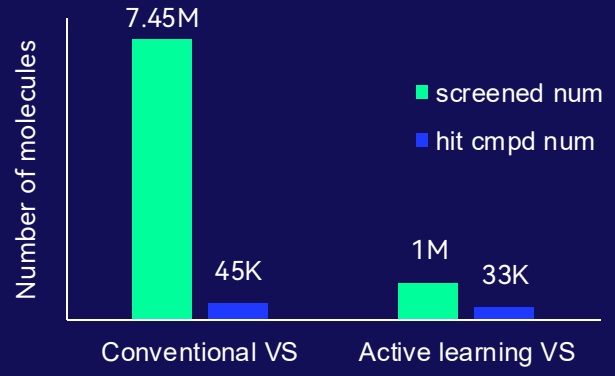
Driving diversity and efficiency with proprietary AI platforms

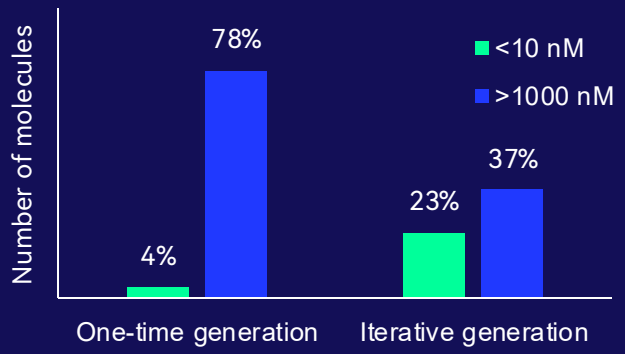
Novel & diverse candidates by generative AI



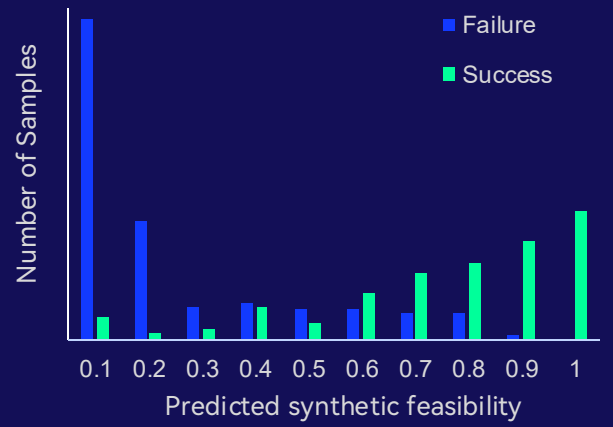


Faster virtual evaluation via active learning





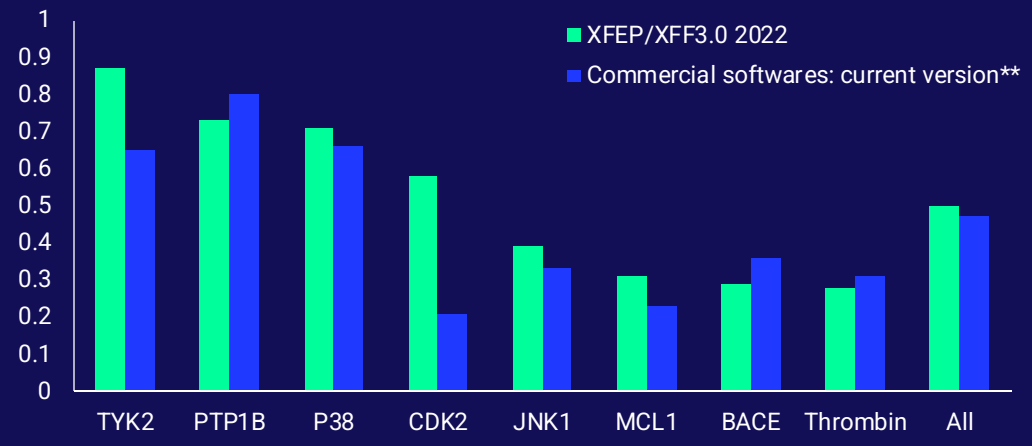
Less trial-and-error for synthesis by predictive AI



- 90% success rate for automated library synthesis feasibility prediction
- 10X synthesis data collection speed for improved synthesis feasibility and protocol forecasting
- ADMET predictive models available

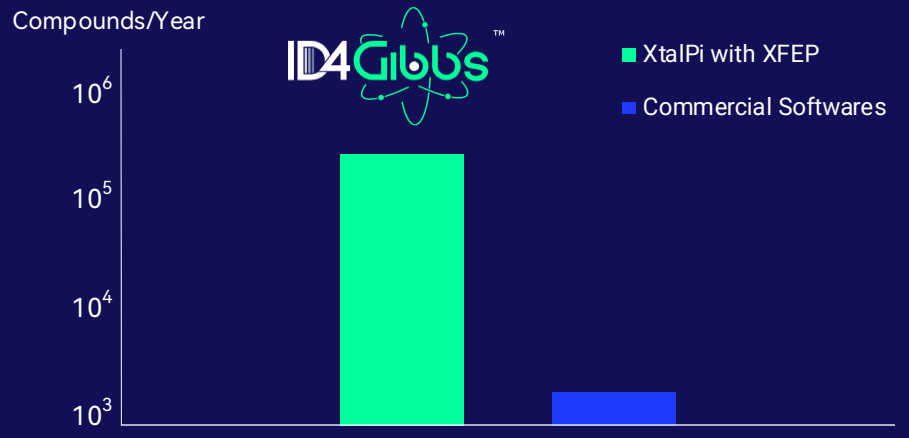
Bolstered efficiency with an accurate, comprehensive, and validated computational chemistry platform

Binding Affinity Prediction Platform with Industry-leading Accuracy (XFEP)



- Validated platform with 30 successful partnerships
- Versatile platform targeting diverse scenarios

Binding Affinity Prediction Platform with Industry-leading Accuracy (XFEP)

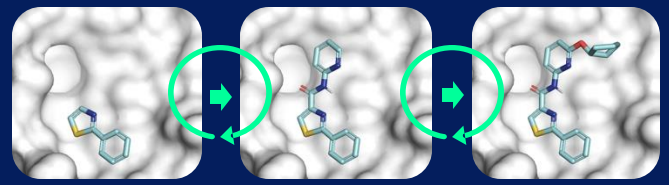


- 80% cost saving, screen more for less
- Superior scalability with cloud-computing

Multi-pronged approach to find hits with the best potentials

VIRTUAL SCREENING

AI-Empowered Fragment Expansion



2 million
Proprietary virtual BBs

10^{12}+
Molecules in XtalPi database

HIGH-THROUGHPUT SCREENING (HTS)

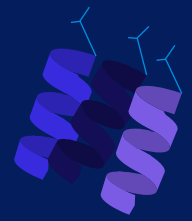
Diverse Classes of HTS libraries

200k+
Drug-like compounds

7.8 million+
Molecules accessible by rapid synthesis

DNA-ENCODED LIBRARY (DEL)

Minimized False Positives by AI recommendation



40+
DEL-compatible chemistry

10^{11}+
Molecules synthesized by DEL chemistry

XtalPi

Small Molecule Drug Discovery

CASE STUDY 1

Best Hits discovery approach focused on accuracy and diversity

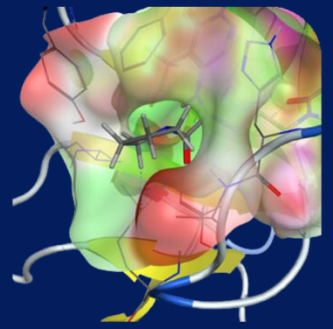
CASE STUDY 2

Applying ID4inno to find potent Hit compounds with novel scaffolds

Best hits discovery approach focused on accuracy and diversity

Challenges

- First-in-class target for which tool compounds are very challenging to identify
- Refinement of the tool compound failed to yield trackable SAR



1 — Round of virtual screening

11M — Compounds from commercial libraries were screened

52 — Compounds recommended by ID4Ideo™ ID4Globus™

2 — HIT CANDIDATES IDENTIFIED
[IC_{50} = 10 nM]
8 compounds with IC_{50} < 5 µM

Automation-empowered rapid analog synthesis in validating hits

HITS RE-TEST
TR-FRET
Dose response

2 HIT CANDIDATES
Re-synthesized
Fully characterized

ANALOGS SAR STUDIES
AI-driven design
Automated synthesis
In 6 days

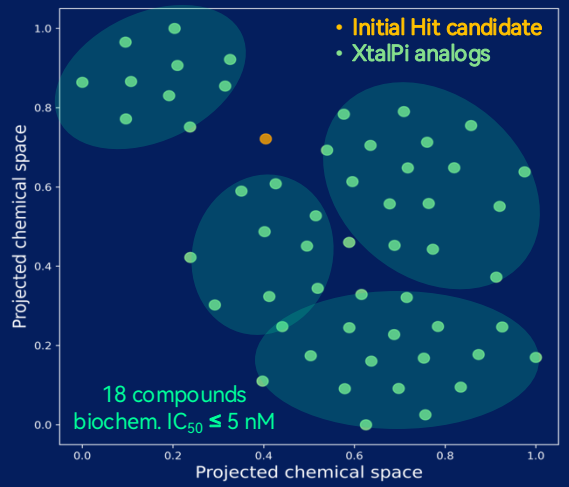
CANDIDATE 1 → 68 Analogs

CANDIDATE 2 → After a few analogs → A False Positive Hit

Early-stage termination through rapid Hit validation

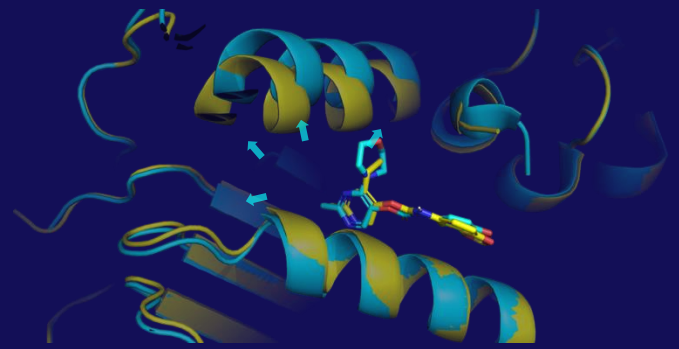
Continue Evaluation of Best Hit

Biochem. (IC_{50})	0.7 nM
Cell (IC_{50})	338 nM
PPB (h)	81%
LMS (h, r, m)	<2, 74, 75 mL/min/kg
CYP (2D6, 3A4M/T)	> 30 mM
hERG	> 30 mM



Rapid Lead-ID for small-molecule inhibitors against a popular oncology target

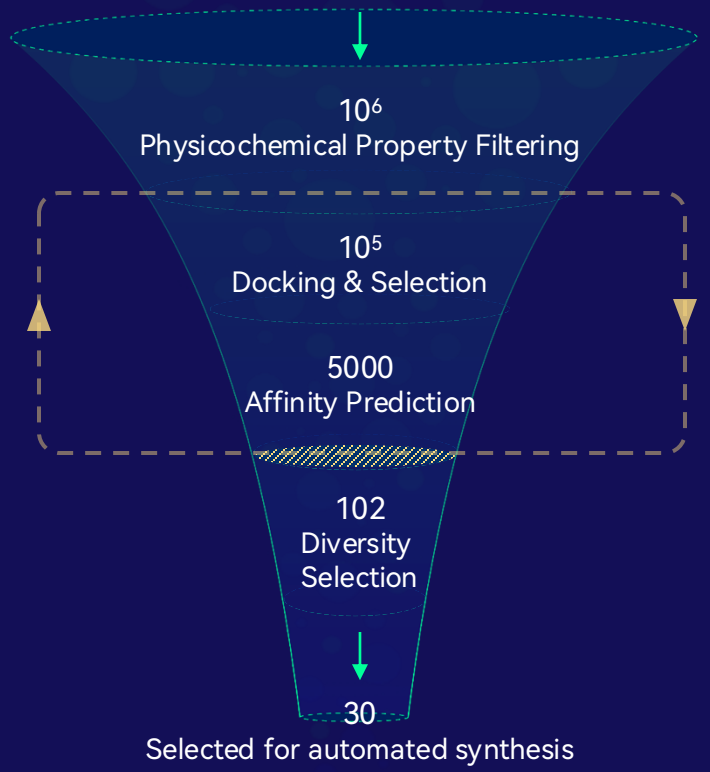
Docking models with compound-1 and compound-2



Challenges

- Allosteric pocket at the junction of highly flexible protein domains
- Pose challenges for accurate computational modeling
- Limited diversity in the initial hits

Molecules from building blocks enumeration by generative AI



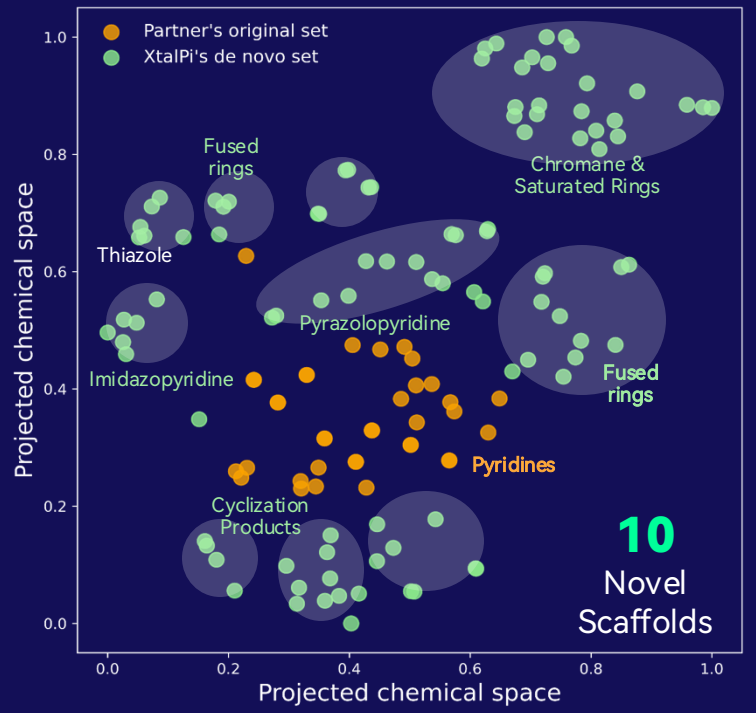
ONE
Month Physics-Based In-Silico work

12
Compounds with potency IC50 < 100 nM

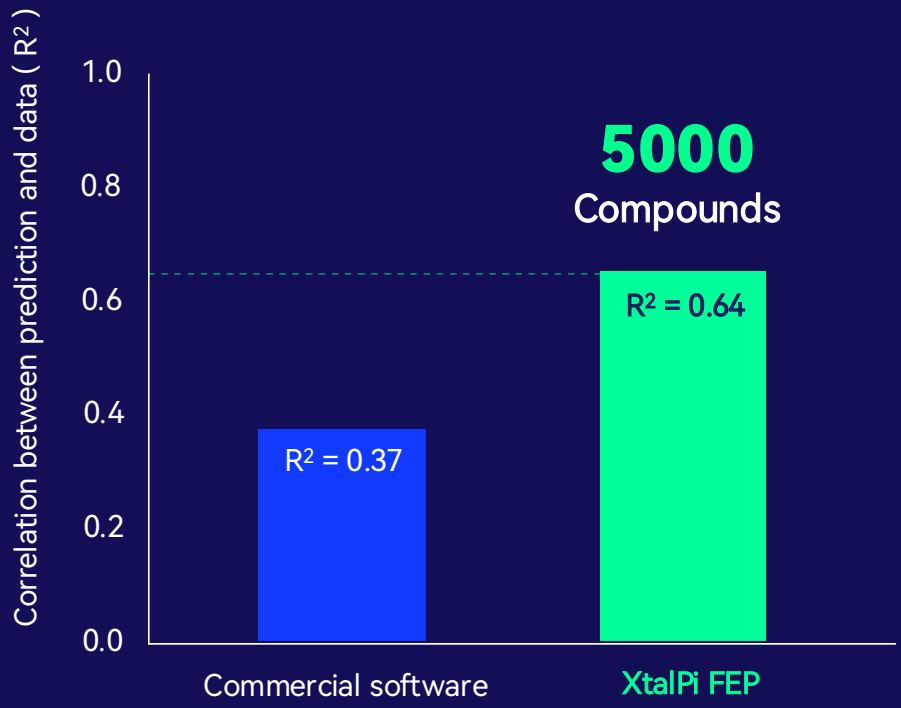
10
Novel scaffolds created by generative AI

Expanded molecular diversity with enhanced efficiency delivered in 1 Month

Broadened Chemical Space with Drug-Like Properties



High-Accuracy Affinity Prediction at Large Scale



XtalPi

Discovery Chemistry Powered by Automation and Digitalization

PART THREE

Rapid discovery chemistry & library synthesis services

50,000 ft²
automated lab space

80%
common Med. Chem. toolbox

200+
workstations

AI-Driven Automation for Revolutionary Chemistry

Crafting the future of chemistry through intelligent software design, data structuring, and automated workstations

SOFTWARE

Core system for experiment operations

- Intelligent scheduling for automation execution
- Data logging & reporting
- In-house design ELN

INTELLIGENT ALGORITHM

Data structing and AI training

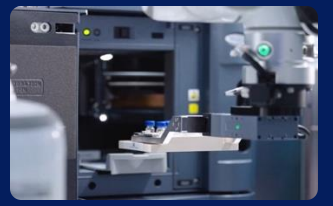
- Rxn. conditions recommendation
- Synthetic process planning
- Substances handling

MODULAR WORKSTATIONS

Automated small molecule synthesis

Glove-box workstations

Precise chemical handler

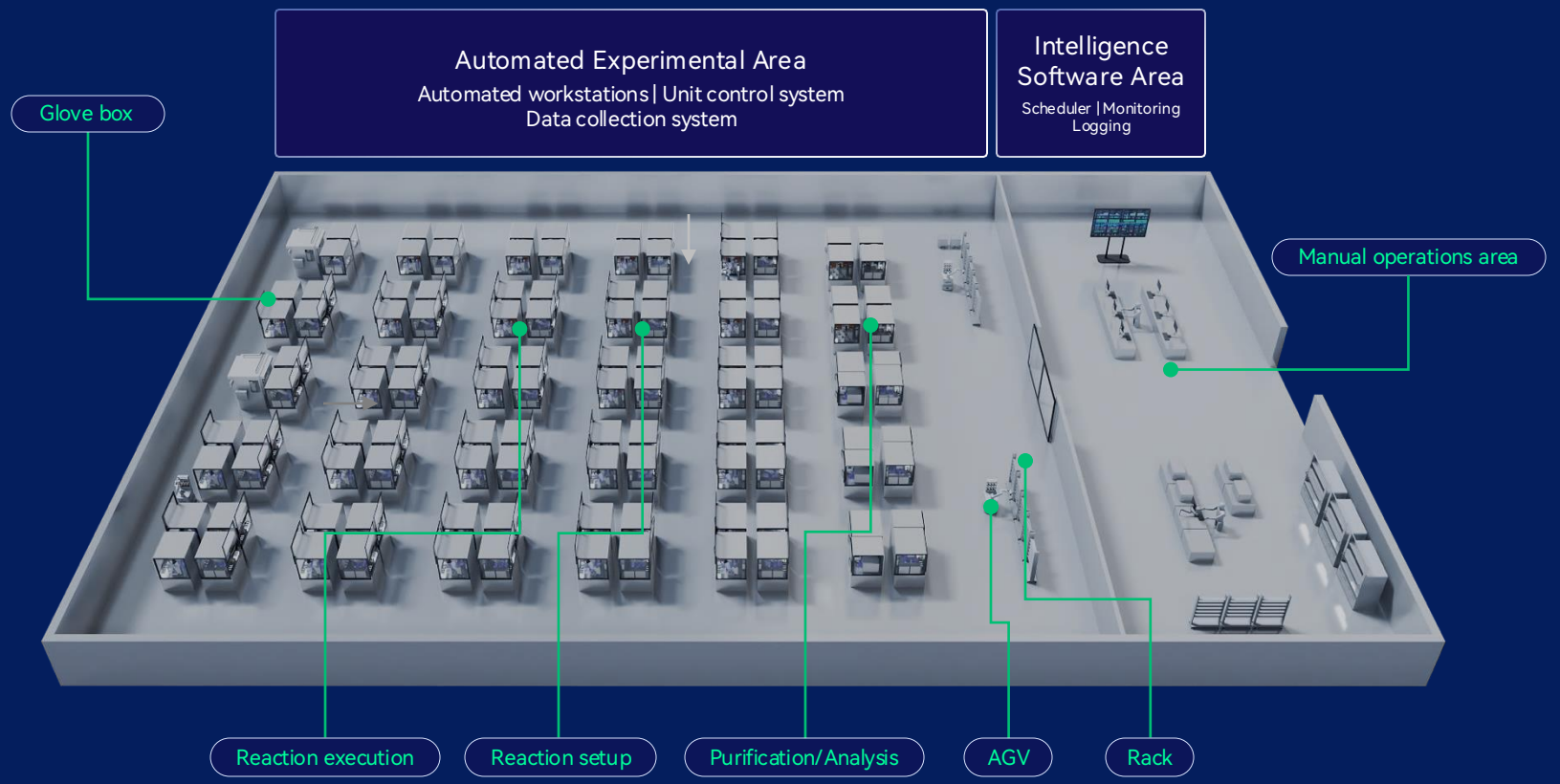


Integrated analytical systems

XtalPi's Cloud-Based Automation Cluster

Integrating precision chemistry execution and intelligent software management for cutting-edge research

Cloud Lab Platform



Scheduling and Controlling System

AI-empowered process control for human-machine interaction (HMI)

Standard Chemistry modules and automated workflows

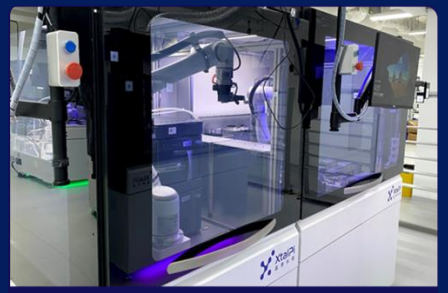
XtaliPi's automation platform covers a range of applications in chemistry

Dispending Workstation

- Solid/Liquid dispending
- Caps opening and closing
- Nitrogen blow

Reaction Workstation

- High-throughput
- Temperature controlled stirring
- Quick sample preparation



Analytical Testing Workstation

- Sample preparation
- LC-MS analysis
- Online report review in ELN

Purification Workstation

- Nitrogen evaporator
- SPE celite columns
- SPE silica gel columns

Glove-box Workstation

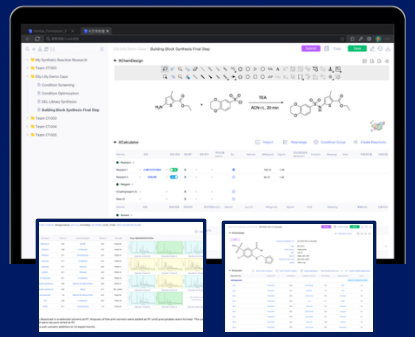
- Reaction operations
- Sample preparation
- High-throughout for moisture and air sensitive reactions

Full digitalization solutions to accelerate discovery

Flexible system and process integration for automation infrastructures of any scale

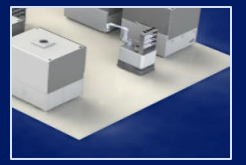
Chemist-Centric ELN

A streamlined ELN and data management for chemistry applications



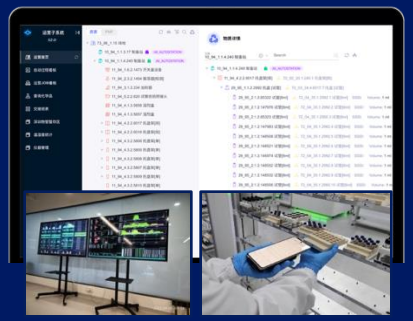
Scheduling and Controlling System

AI-empowered process control for human-machine interaction (HMI)



LIMS

Resource and quality management with a focus on automation cluster



Digital Twins System

Planning tools for process optimization and lab/experiment design validation

Break free from chemistry bottleneck with intelligent scalable automation

up to 50%
enhanced speed

Rapid Library Synthesis
with superior compound novelty & diversity

Accelerate hits and leads discovery via bespoke library synthesis

FOCUS LIBRARY

Target-focused

- Synthesize the libraries designed by XtalPi or Partner
- Main scaffold and building blocks by partner or XtalPi
- Bioassays by request
- Rapid reaction

FIXED LIBRARY

Therapeutic areas and/or modality-specific

- XtalPi designs and synthesizes library
- Main scaffold and building blocks by XtalPi using generative AI
- XtalPi offers enumeration
- Partner owns the right to select final compounds

Enabling discovery chemistry with flexible offerings

Full-Time Equivalent (FTE)

- Flexible team sizes
- Agility to targets or project reprioritization

Fee for Services (FFS)

- Premium compound synthesis available form mg to kg scale
- Pay for successfully delivered compounds

Chemical Synthesis

- Final compound synthesis
- Building block synthesis
- Library synthesis
- Intermediate/scaffold synthesis
- Reference standard synthesis
- Synthetic routes design and scouting
- Reaction condition optimization
- Catalyst screening
- Custom synesis
- Chiral SFC separation

Customized Synthesis

- Peptides
- PROTAC
- ADC
- Macrocyclic compounds
- Stable-isotope labeling chemistry
- PhotoRedox Catalysis

XtalPi

Automated Discovery Chemistry

CASE STUDY 1

Reaction conditions screening

CASE STUDY 2

Rapid, parallel compound library synthesis

Accelerating DMTA based on AI and automation infrastructure

AI & COMPUTATION

1

Focused Library
Property predictions
Synthesizability

75

3rd Day
In-Silico Completed

Recommended Compounds
Building blocks of un/cyclized and/or 1°/2° amines

AUTOMATED SYNTHESIS

150

Automated Reactions
2-step synthesis
Selective amide coupling

68

6th Day
Synthesis Completed

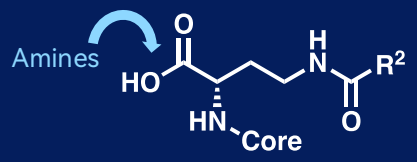
Target Molecules Delivery
Up to 80% overall yield
Purity ≧ 95%

IN-HOUSE BIOASSAYS

6

7h Day
Biology Completed

Potent Compounds
FRET IC_{50} < 2 nM
Fast SAR exploration



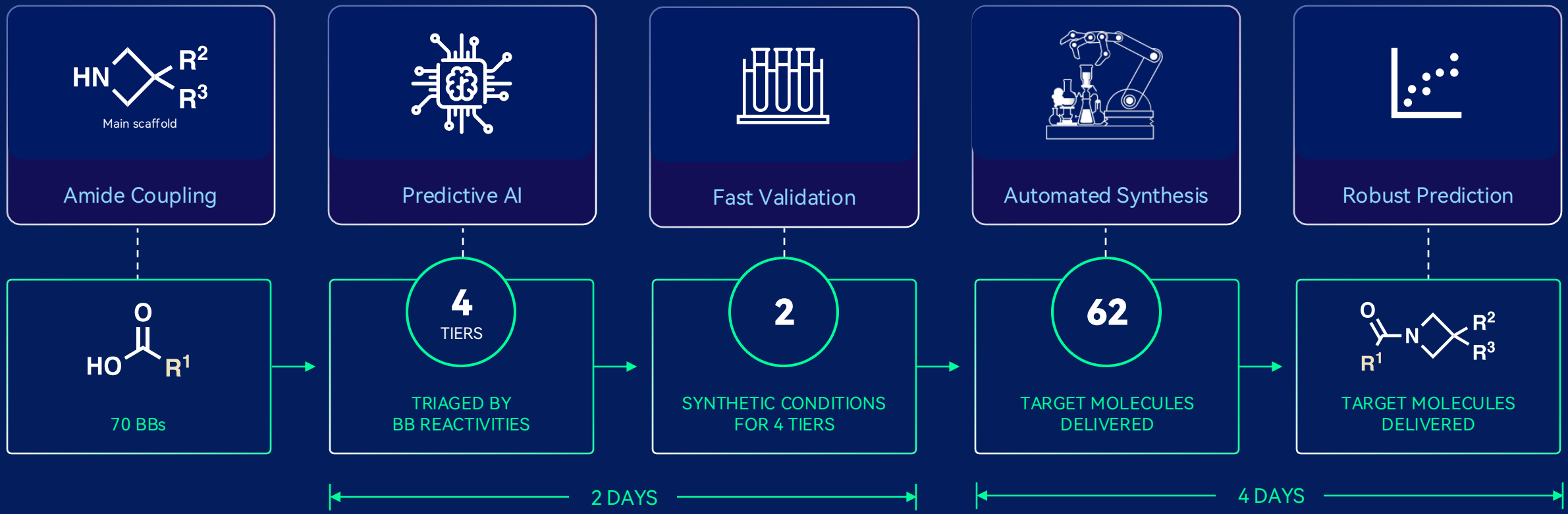
57,721
Molecules enumerated

7
Workdays

91%
Overall success rate

Rapid library delivery in 6 days by synthesizability assessment

Reaction conditions recommended by AI based on predicted building block reactivities to enable rapid library synthesis



XtalPi

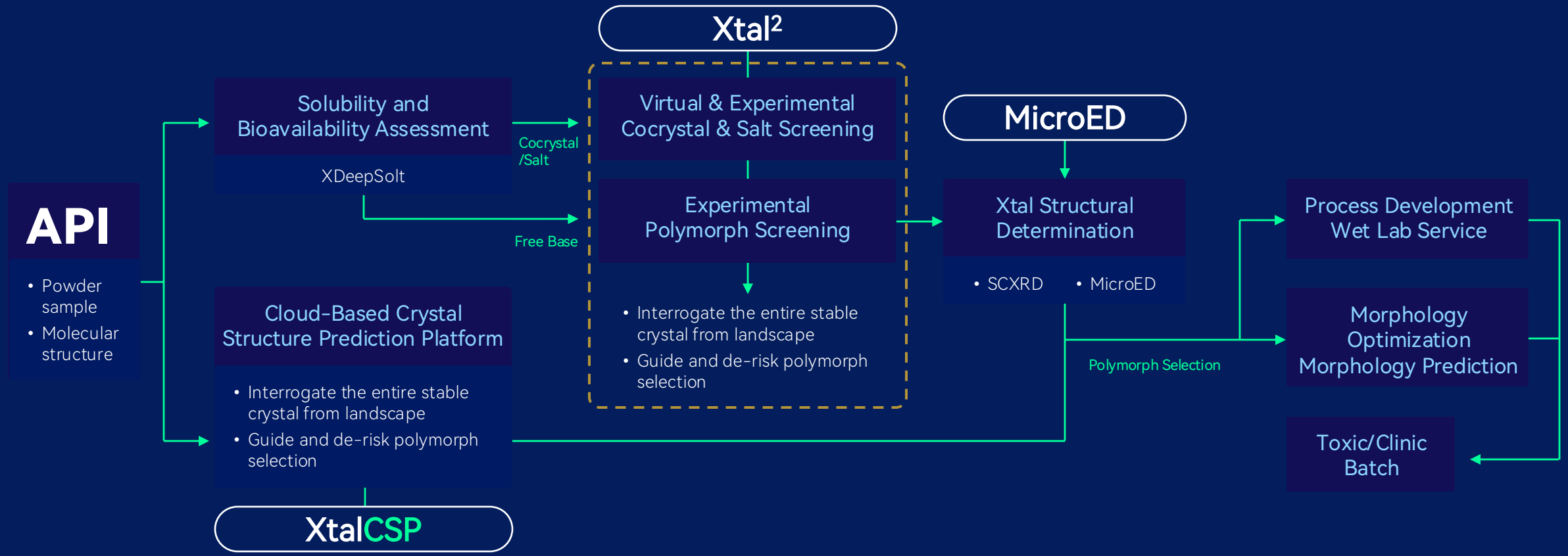
Solid-State Platform for Drug Formulation Development

PART FOUR

Rapid discovery of the desired form for formulation development

Multi-pronged, risk mitigated approach that harnesses the power of proprietary AI algorithm, quantum physics, and automation.

- Survey the complete stable crystal landscape
- Design experiments smarter
- Screen polymorphs faster
- Make decision under unparallel timelines



Advantages of XtalPi sold state platform

High Quality

EXPERTISE & SPECIALTY

- Demonstrated experience and computational empowerment
- Definite results by CSP with 98% coverage

Speedy Delivery

QUALITY & EFFICENT

- 25%-50% increase in delivery speed
- Commitment to delivering high-quality results, fast

Cost Effective Solution

FLEXIBLE & TAILORED APPROACH

- Tailor the proposals to meet diverse needs
- Flexible to the requirements of timeline and budgets

Cutting-Edge Tech

INNOVATION

- Focus on scientific innovations
- Proprietary prediction, automation and MicroED platforms

Comprehensive, flexible solid-state solutions

Intelligent

EXPERIMENTAL SOLID-STATE & FORUMATION SERVICES

- Polymorph/salts/cocrystal screening and selection (empowered by AI-guided condition strategy)
- Crystallization process development
- Solid dispersion formulation development
- Analytical method development
- Pre-formulation development

Industry-Leading

COMPUTATIONAL STRUCTURAL PREDICTION SERVICES & PLATFORM

- Crystal structure prediction
- Virtual salt/cocrystal screening
- Solvate/solid dispersion propensity prediction
- Moorphology prediction
- Access to our XtalCSP computational platform (coming soon)

Rapid

CRYSTAL STRUCTURE DETERMINATION

- Single crystal preparation and structure determination
- Rapid crystal structure determination using in-house MicroED analysis

Fast, versatile, cloud-native solid-state R&D platform

Advanced solid-state computational services

COMPUTATION PLATFORMS

CSP

XtalCSP

Crystal structure prediction to fully de-risk the system

CSP - Lite

CSP-LITE

Fast crystal structure prediction

Virtual Screening

VIRTUAL COFORMER

Perform virtual screening between API and conformers (counter ions)

MP

MORPHOLOGY PREDICTION

Predict the morphology of target polymorph in solvents

COMPUTATION & DATA INFRASTRUCTURE

 Cloud computing platform

 Data center

 Quantum physics

 AI + machine learning

Xtal2 Proprietary AI-driven polymorph strategy

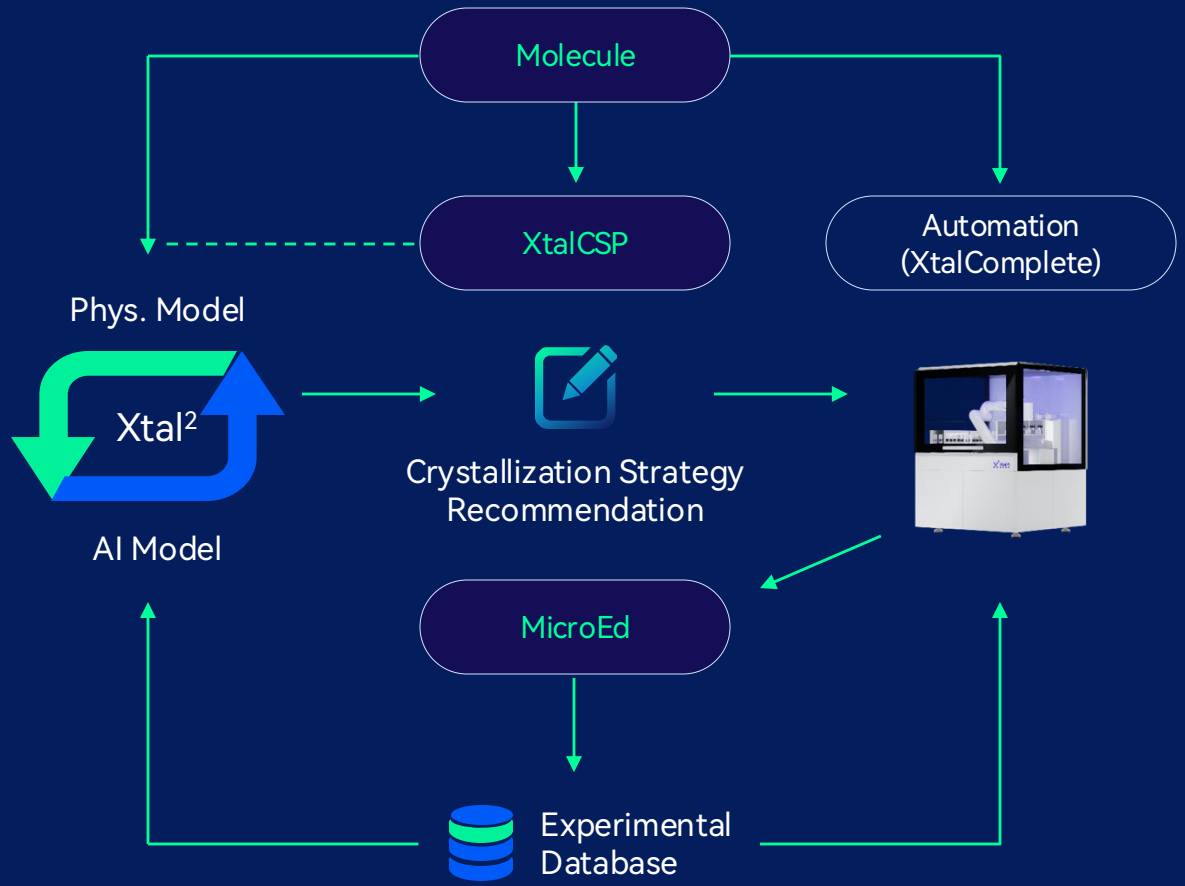
Xtal2 combines physical-based (virtual) data and real-world crystallization results to perform virtual screening, significantly increasing the screening efficiency of polymorphs including salt and co-crystal

Crystallization condition recommendations

- Crystallization methods and conditions
- Conformer and counterion and solvent

Breaking limitation of human bias in experimental design

- 80%+ powder yield
- Significantly reduce sample consumption and accelerate experimental cycles



XtalPi

Solid-State Platform for Drug Formulation Development

CASE STUDY 1

Accelerate solid form selection

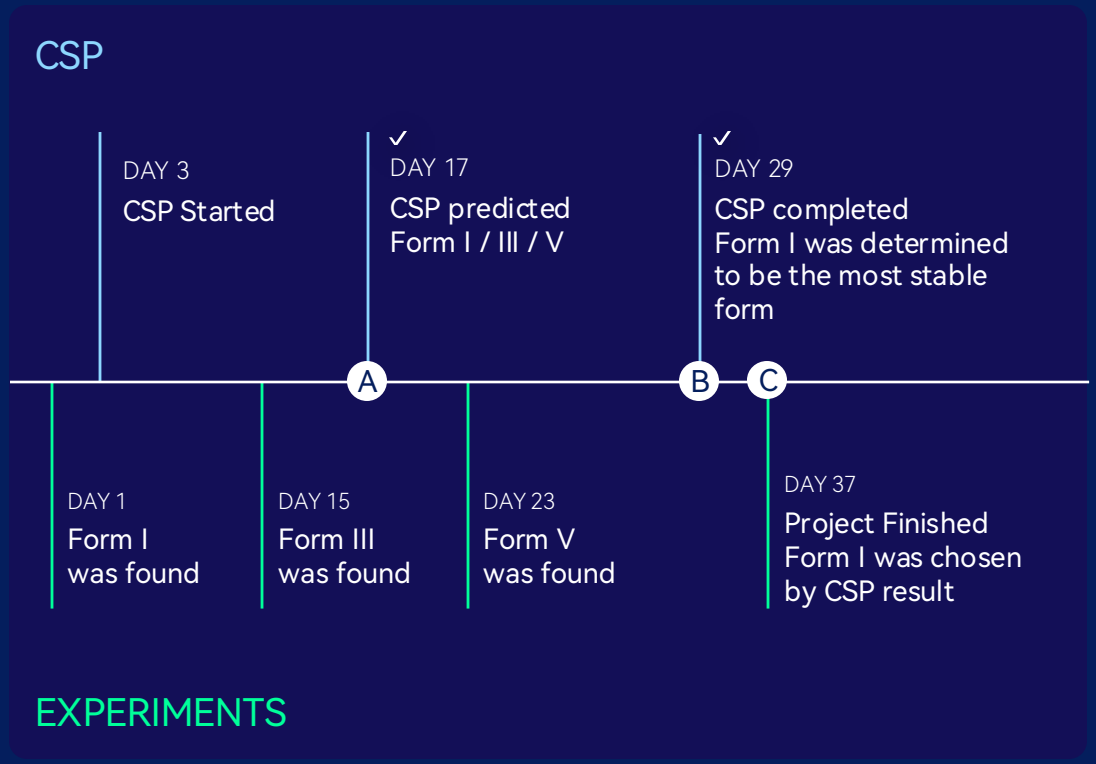
CASE STUDY 2

Polymorph screening guided by AI and accelerated by automated crystallization platform

XtalPi CASE STUDY 1

Accelerate solid form selection

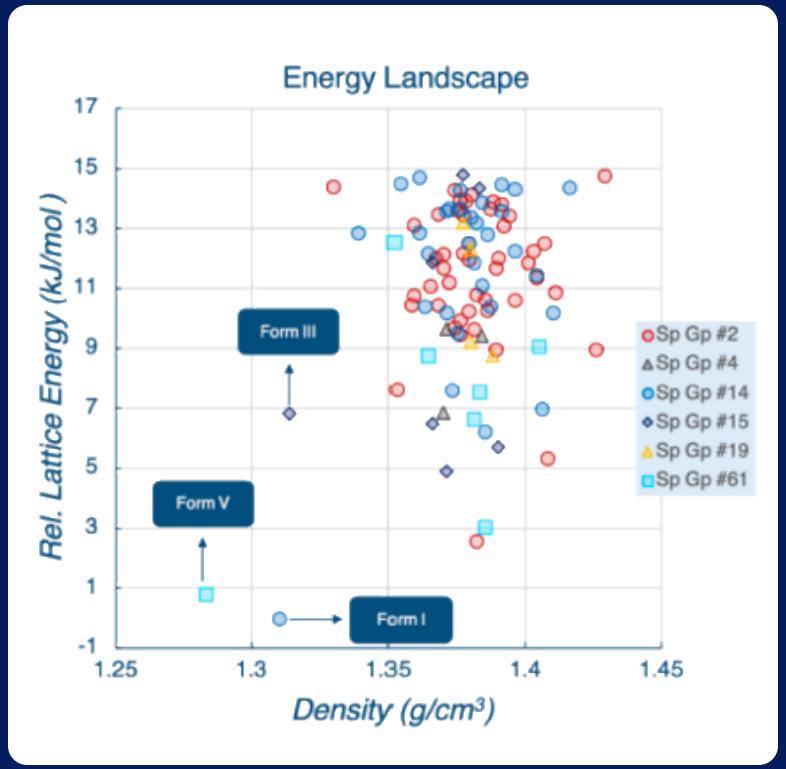
Determining a solid form needed for a clinical study in two months by leveraging a combination of XtalPi's CSP platform and experiment methodologies.



A Found potential polymorphs other than Form I; results guided further experimental screening

B Thermodynamic stability calculation lowered decision-making risk

C Time needed for decision-making was shortened given confirmative CSP results



XtalPi CASE STUDY 2

Polymorph screening guided by AI and accelerated by automated crystallization platform

Achieving quality-results under an accelerated timeline using XtaliPi intelligent approach

1 ×

200
Manual experiments designed by experts

3.5
weeks

4.0g
sample

# of exp.	# of solids obtained	Hit Rate	# of discovered forms
200	174	87%	3

≤

0.4 × 1 ×

70
automated experiments guided by intelligent crystallization strategy

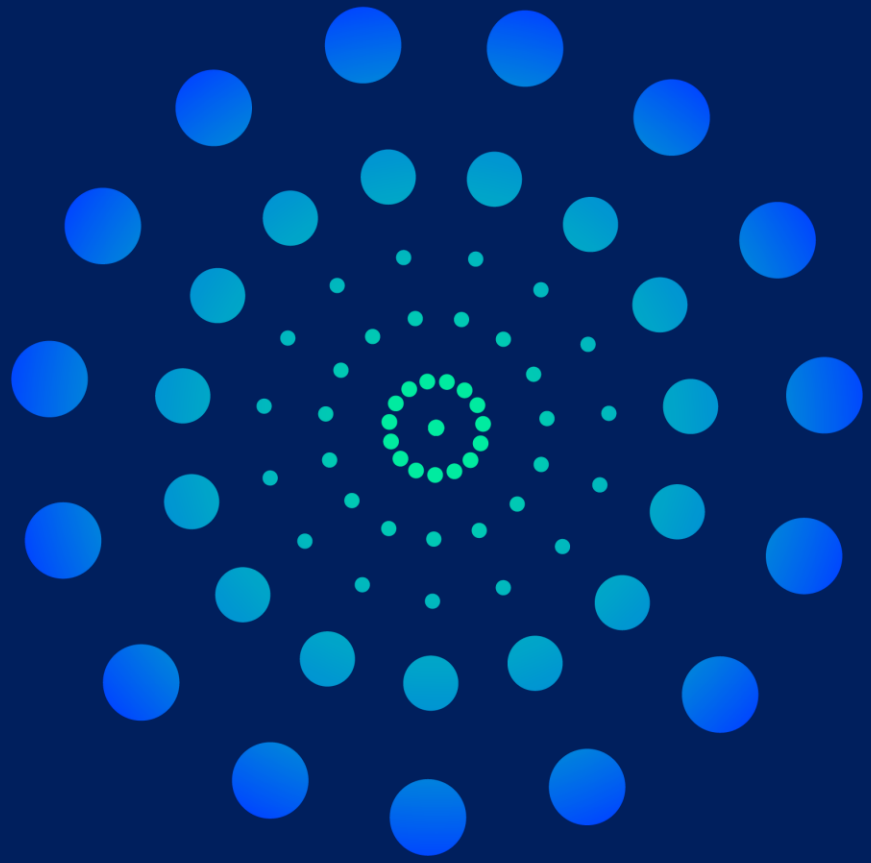
2
weeks

1.5g
sample

# of exp.	# of solids obtained	Hit Rate	# of discovered forms
70	64	92%	3

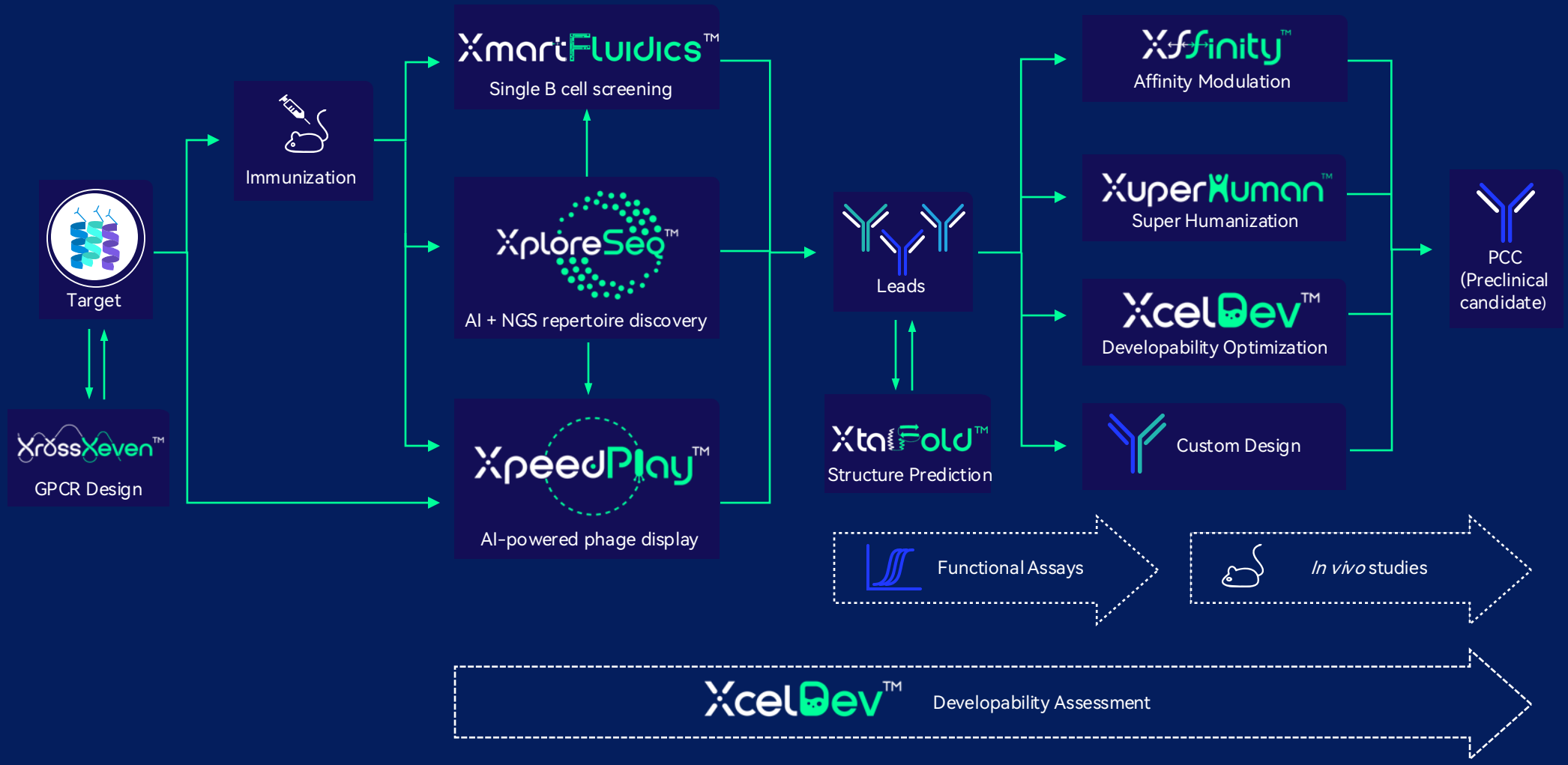
XtalPi

Antibody Discovery

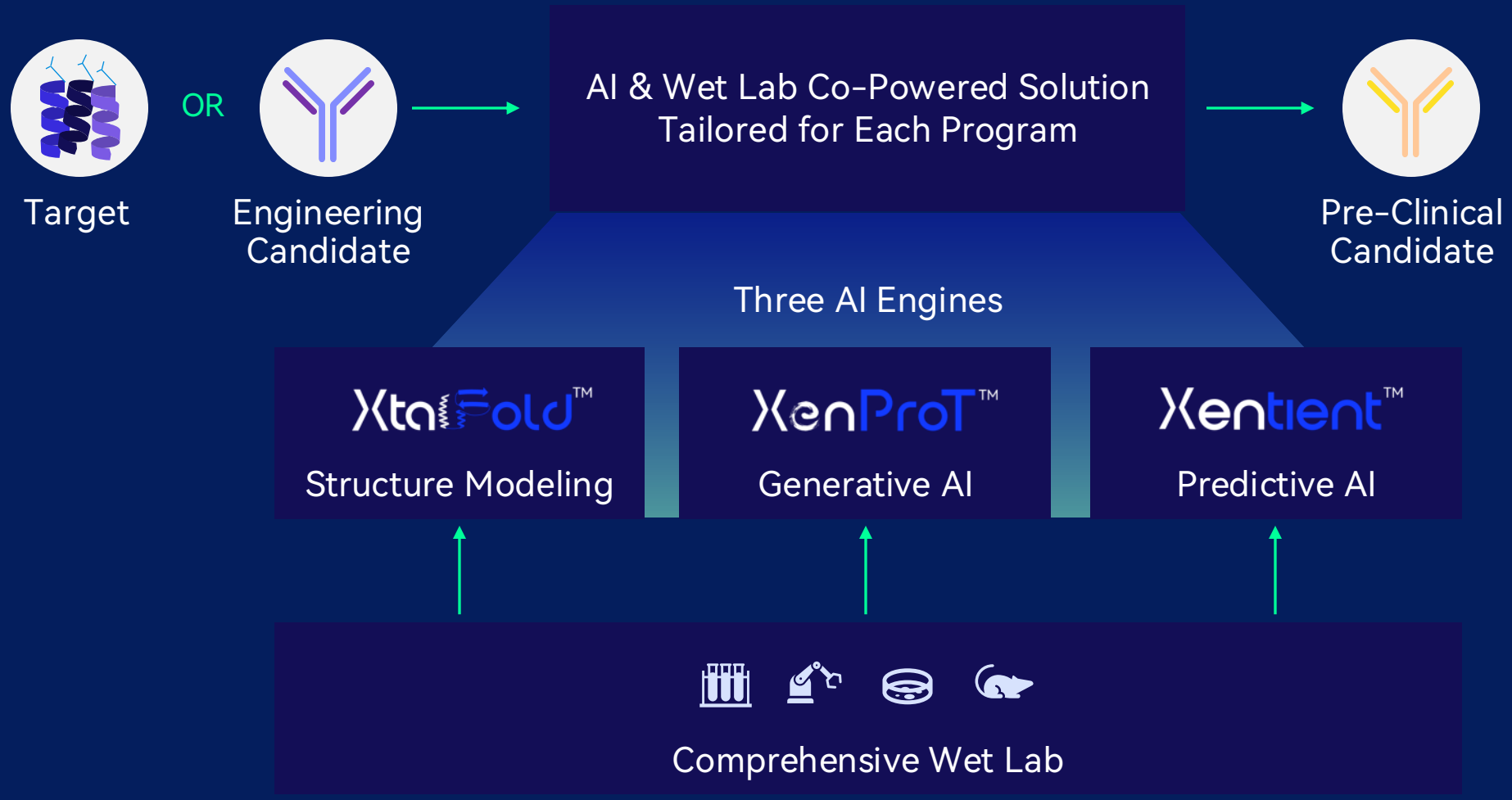


PART FIVE

Overview of our antibody discovery platforms

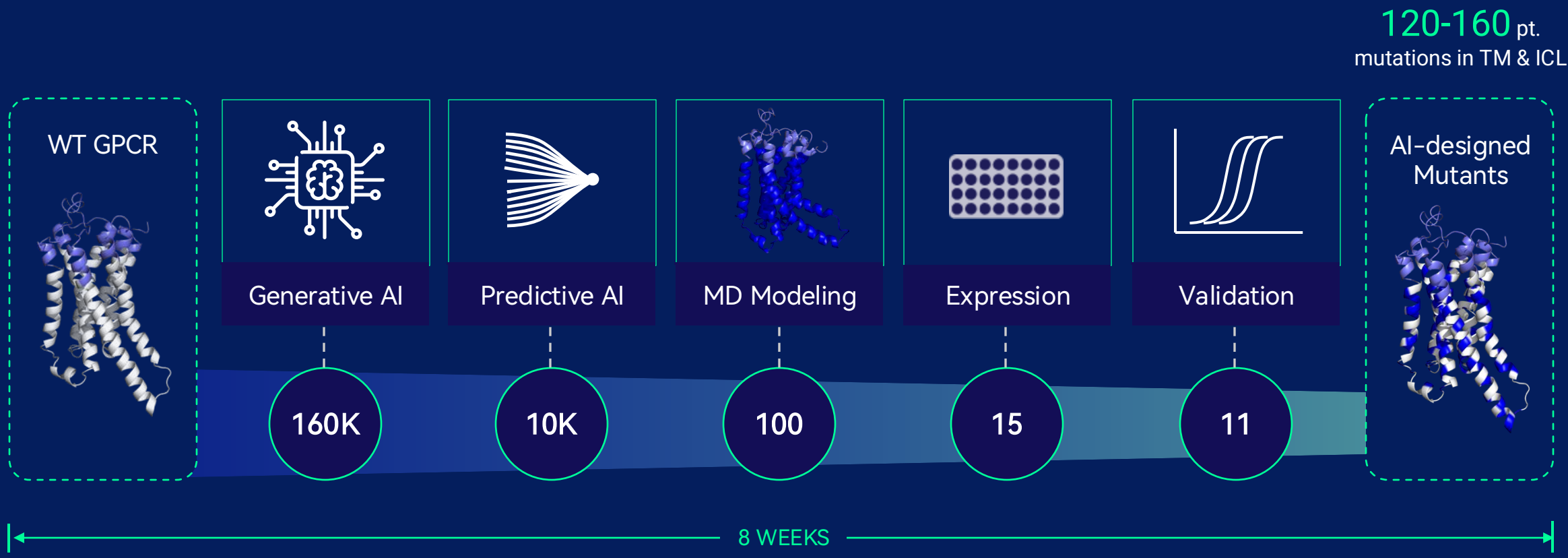


Our Tech Stack



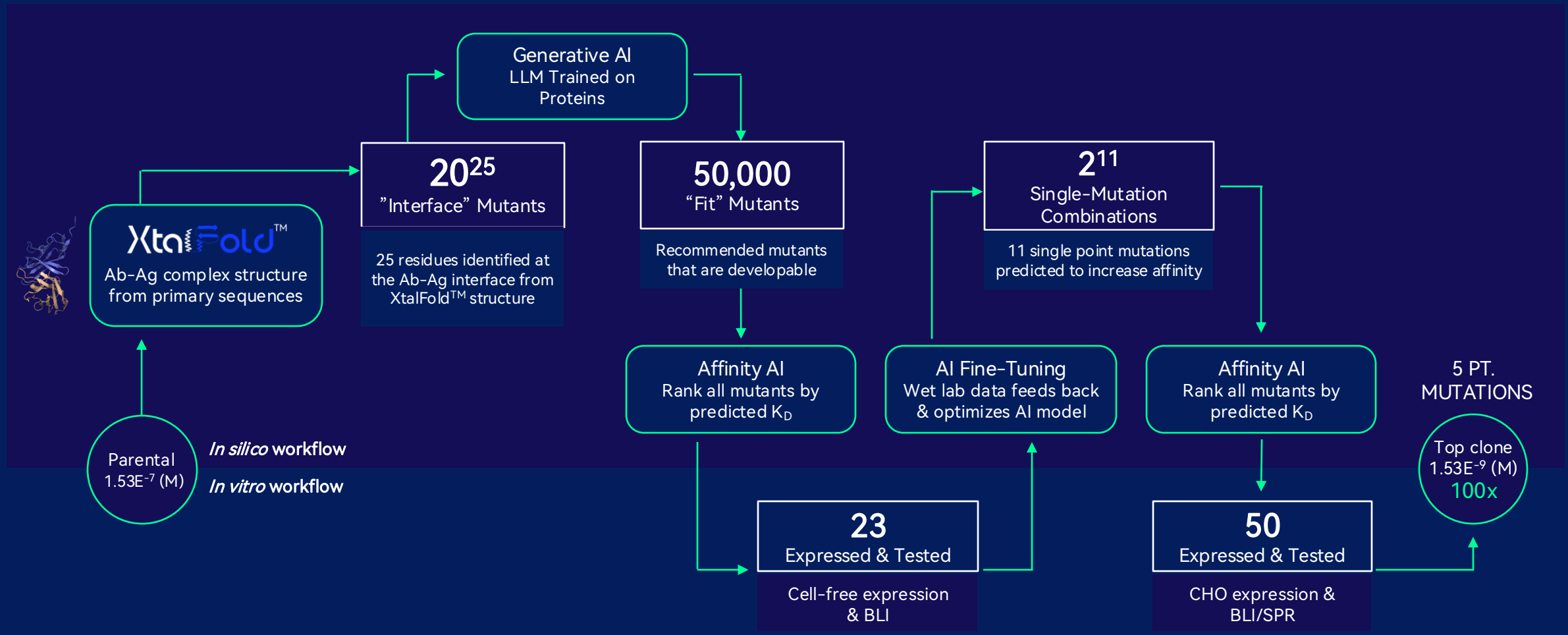
Generating antibodies through AI-designed GPCR antigen

Hard-to-express GPCR antigen acquired after AI-driven large-scale mutations



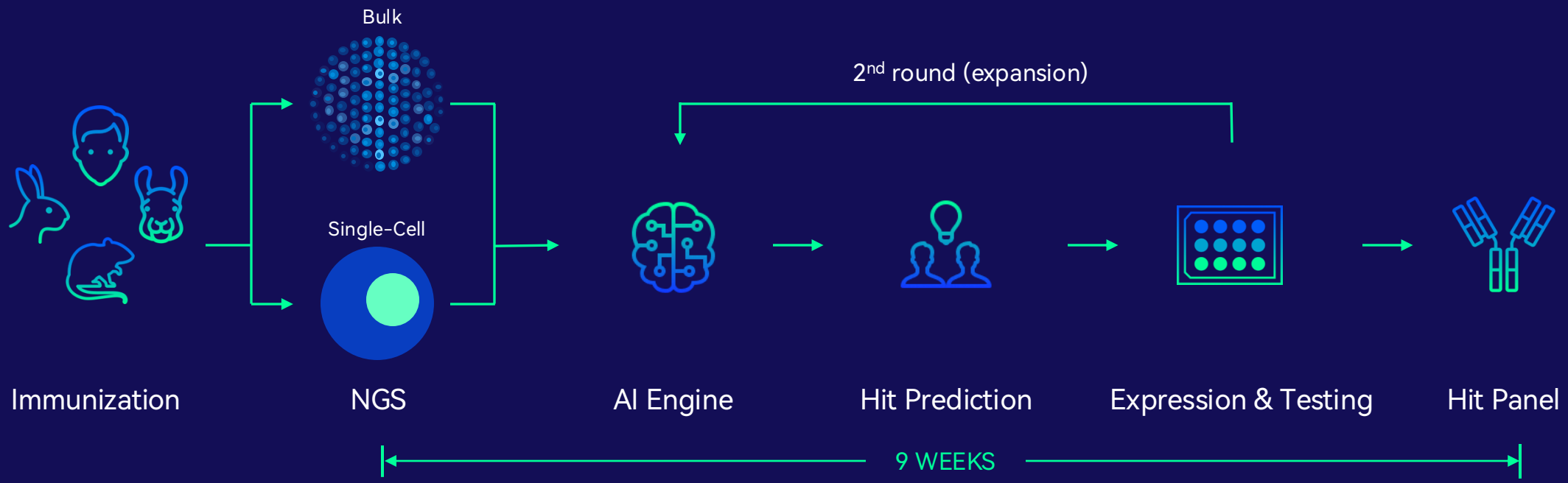
Ultra-fast AI-guided affinity maturation

2 Rounds of Optimization | **73** Variants Expressed | **3.5** Weeks | **100x** Increase in Affinity



NGS +AI to rapidly generate a diverse panel of functional and developable candidates

FAST | DIVERSE | DEVELOPABLE | HIGH HIT RATE



XtalPi

Confidential Copyright

Unauthorized use of this document's information, owned by Shenzhen Jingtai Technology CO., Ltd., is prohibited, legal action pursued against violators.