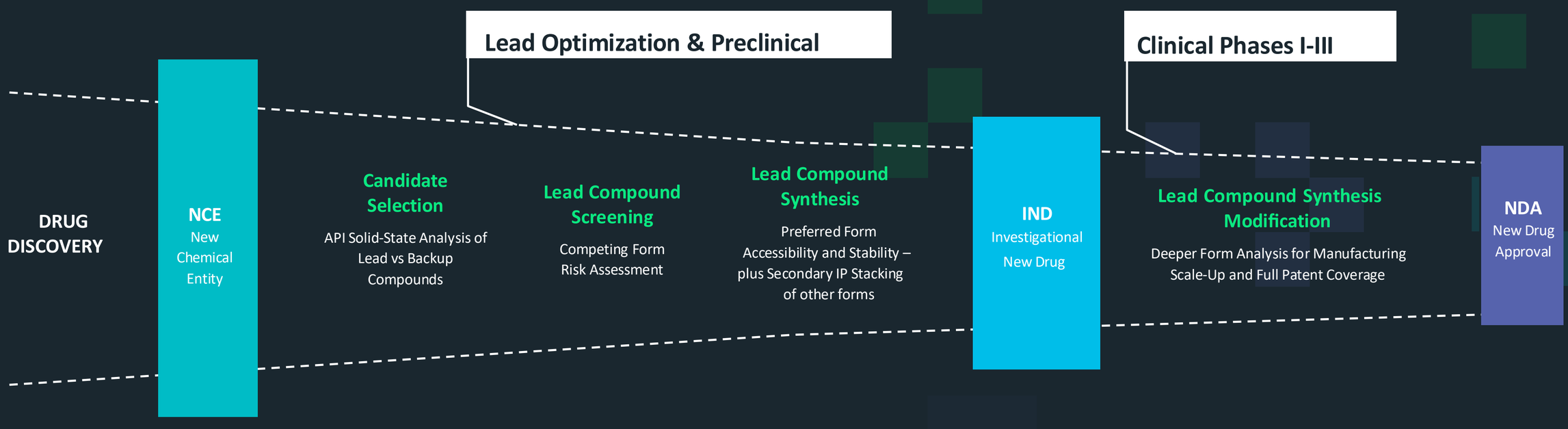
biosimulytics

Your *in silico* solid-state partner

Know your polymorph risks – the earlier, the better

Prediction + Lab : add powerful predictive insights early, and at key intervals, to enhance and guide your experimental results



BiosimX CSP Modular Suite – accessible for all Labs

Flexible gated approach – tailor the solution to suit your development phase needs, budget and timelines

CANDIDATE SELECTION

COMPETING FORM RISK ASSESSMENT

PREFERRED FORM ACCESSIBILITY AND STABILITY

DEEPER FORM ANALYSIS FOR MANUFACTURING & PATENTING

Fast CSP

~72% landscape coverage*

Module BSX-01

Z'=1 90%
MLIP - based

Enhanced CSP

~81% landscape coverage*

Module BSX-02

Z'=1 99.9%
DFT-based

~92% landscape coverage*

Module BSX-03

Z'=2 90%
pseudosym
DFT-based

~95% landscape coverage*

Module BSX-04

Z'=2 90%
non-pseudo
DFT-based

Full CSP

~96% landscape coverage*

Module BSX-05

Z'=2 99%
pseudosym
DFT-based

~97% landscape coverage*

Module BSX-06

Z'=2 99%
non-pseudo
DFT-based

Flexible Add-On Options

Module BSX-10
Harmonic
Free Energy

Module BSX-09
Solvent Choice
Guidance

Module BSX-08
Symmetry Breaking
Z'>2 Exploration

Module BSX-07
Free Energy Analysis
Using High Fidelity DFT

- Build your dataset coverage incrementally as you go
- Easily integrated into your CMC workflow
- Combine with experimental results at key intervals to make smarter decisions for your development pathway

*Statistical coverage based on data for enantiomerically pure crystals of chiral organic molecules in the Cambridge Structural Database (CSD, Version 5.46)