

Small Molecule Design Engine

CarbonAI™

MODULES



MOLECULE GENERATION

Scaffold Hopping de novo Generation
Lead Optimization Analog Expansion
PROTAC de novo Generation



GENERAL PHARMACOLOGICAL PROFILE OPTIMIZATION

ADME (Absorption, Distribution, Metabolism, Excretion) Prediction
Toxicity Prediction
DMPK Prediction



TARGET BINDING AND SELECTIVITY OPTIMIZATION

Protein Pocket Binding Affinity Prediction
Protein Sequence Binding Affinity Prediction
Target Binding Pocket Detection
Molecular Docking



COMPOUND OFF-TARGET PREDICTION



APPLICATION SCENARIOS

Target Selectivity Optimization
Multiple Pharmacology Profile Optimization
Chemical Reagent Property Optimization

WHY CHOOSE AINNOCENCE?

No Structure Required
Wet Lab Validated
Super High Throughput
Fast: Hours To Days

GREAT TRUTHS ARE ALL SIMPLE

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