CarbonAI®

Small Molecule Design Engine

Lead Generation

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

Lead Optimization

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

Target Binding Optimization

- Protein Binding Specificity Optimization
- Target Binding Pocket Detection
- Molecular Docking

Off-Target Prediction

- Compound Off-target Toxicity Prediction

Application Scenarios

Target Selectivity Optimization

Multiple Pharmacology Profile Optimization

Chemical Reagent Property Optimization

Why Choose Ainnocence?

1. No structure required
2. Wet-lab validated
3. Ultra-high throughput
4. Rapid Turnaround: from a few hours to two weeks

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