



아주대학교 양자-AI 분자설계 연구실

Quantum-AI Molecular Design Lab.

Since 2026. 09

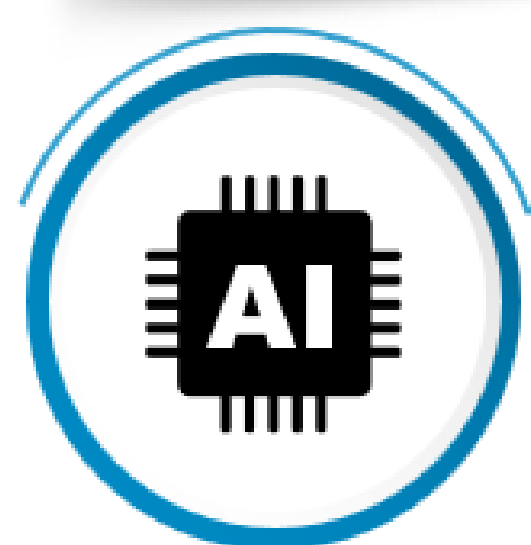
양자-AI 분자설계연구실은 양자화학과 인공지능을 융합하여 화합물 및 단백질 기반의 신약·신소재를 설계하고 검증하는 전산 플랫폼 기술(Q-SAGE)을 연구합니다.



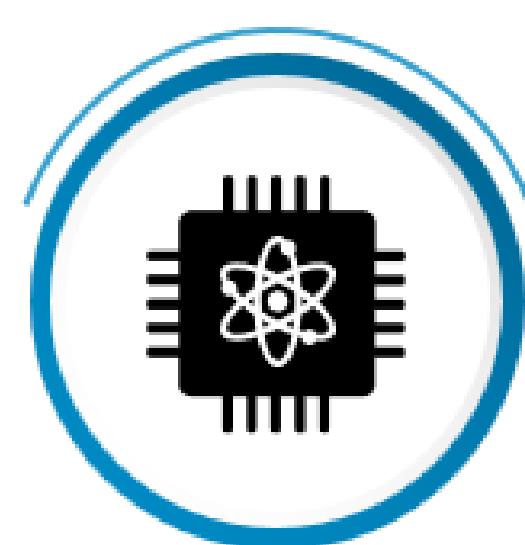
Scoring-Assisted
Generative Exploration

Q-SAGE: Quantum-AI driven Molecular Design

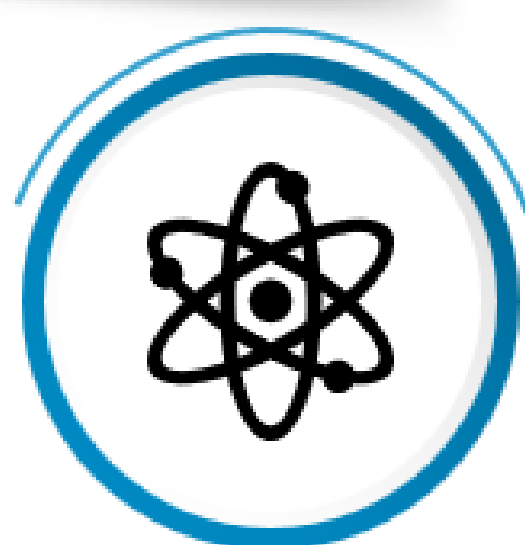
Quantum-AI Molecular Design



Gen : Generative AI
(SAGE, SAGE-Prot)



Eval : Property Pred.
(Quantitative SAR)



Val : Quantum Chem.
(Fragment MO)

Scoring-Assisted Generative Exploration (SAGE)

Education

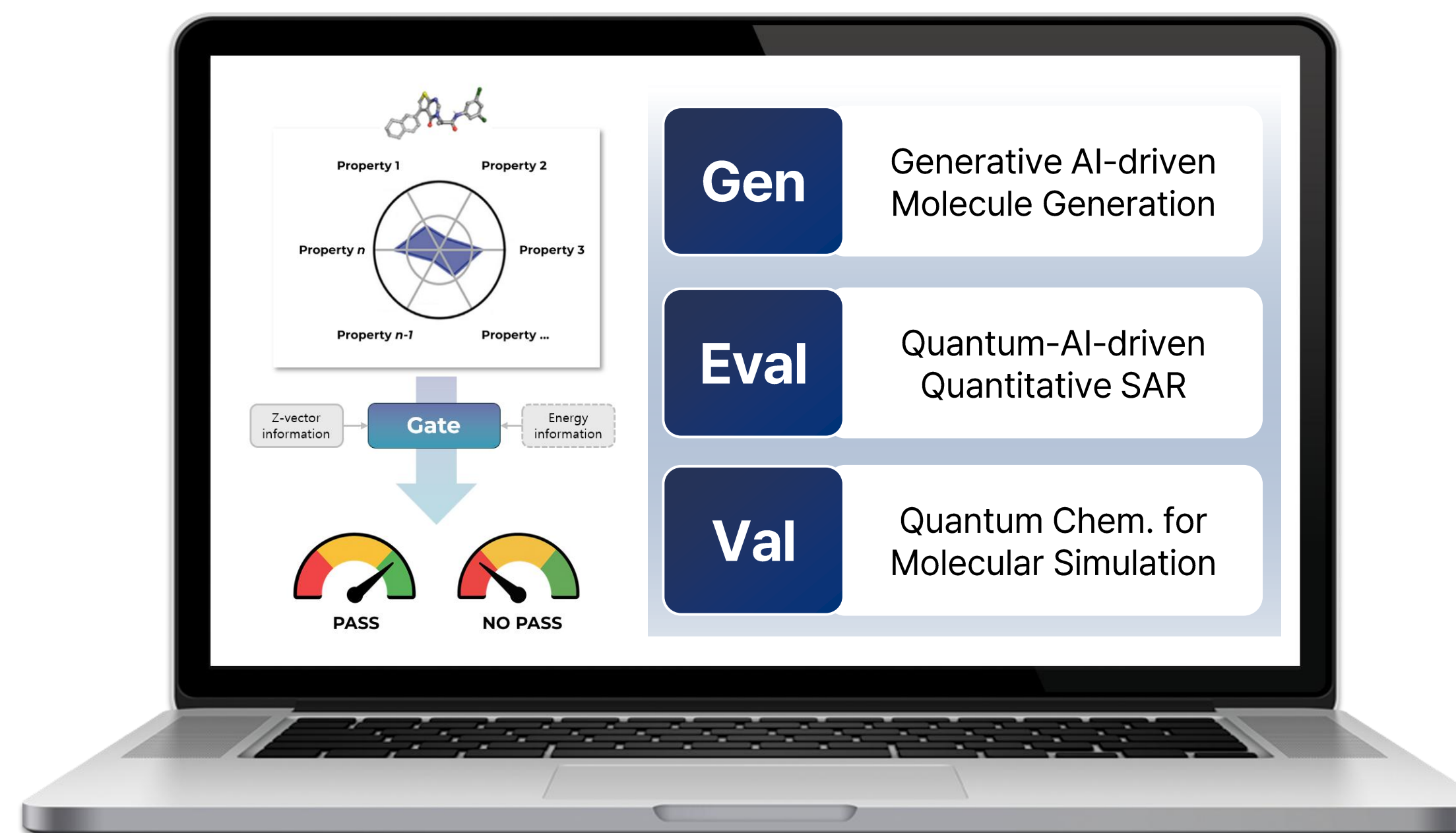
- Interdisciplinary Digital Biology
- Quantum-AI-BIO Molecular Design

Research

- SAGE & SAGE-Prot Molecular Generation
- Quantum-AI driven Accelerated Discovery**

Project

- Quantum-AI-BIO Integrated Projects
- Platform Tech. Accelerated Study



양자-AI 분자설계연구소 (Q-SAGE)

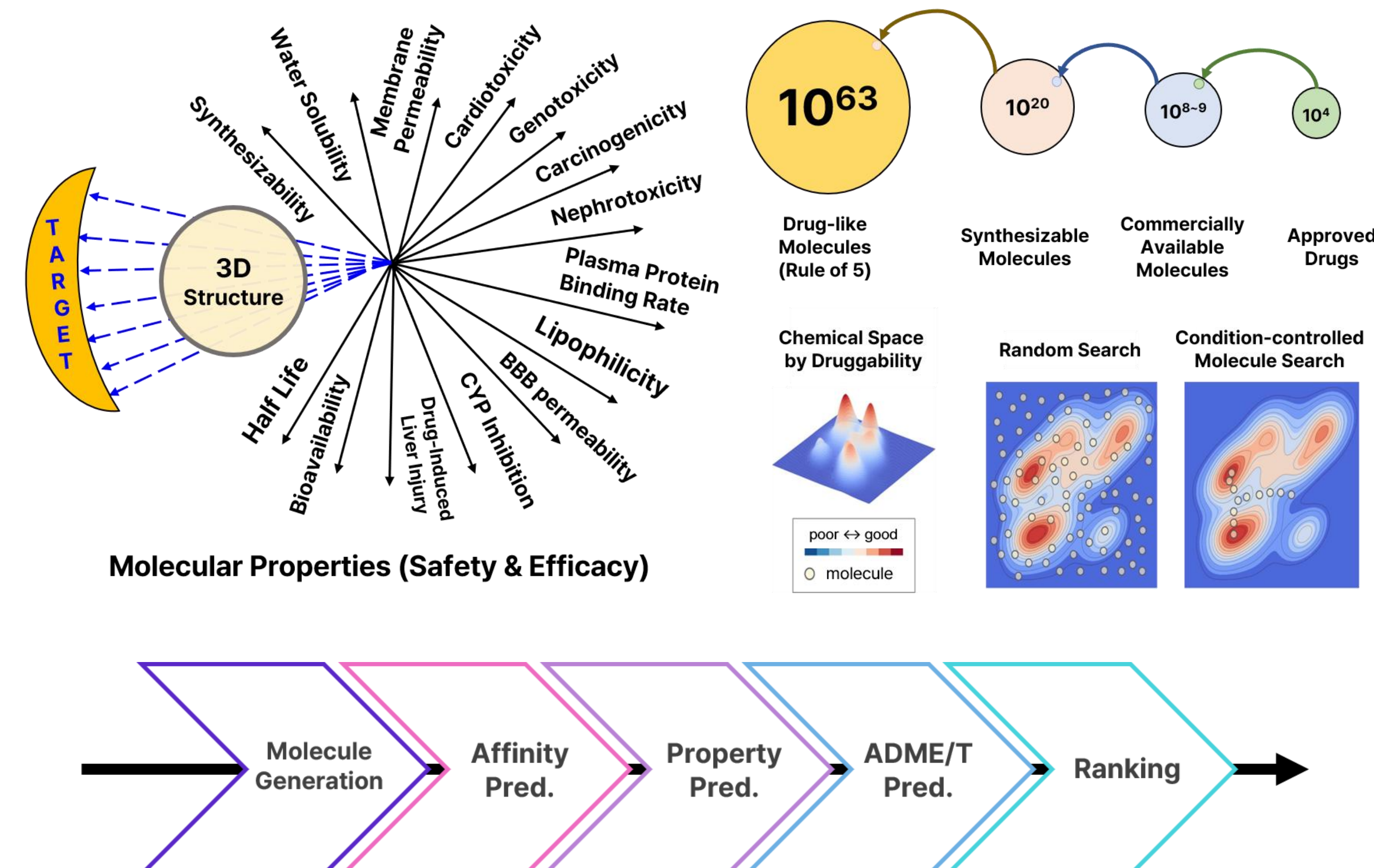
- 생성형 AI와 양자화학 시뮬레이션 기반 통합 분자 설계 플랫폼
- 데이터 기반 탐색과 물리 법칙 기반 검증을 결합한 신약·신소재 발굴

핵심 연구 파이프라인

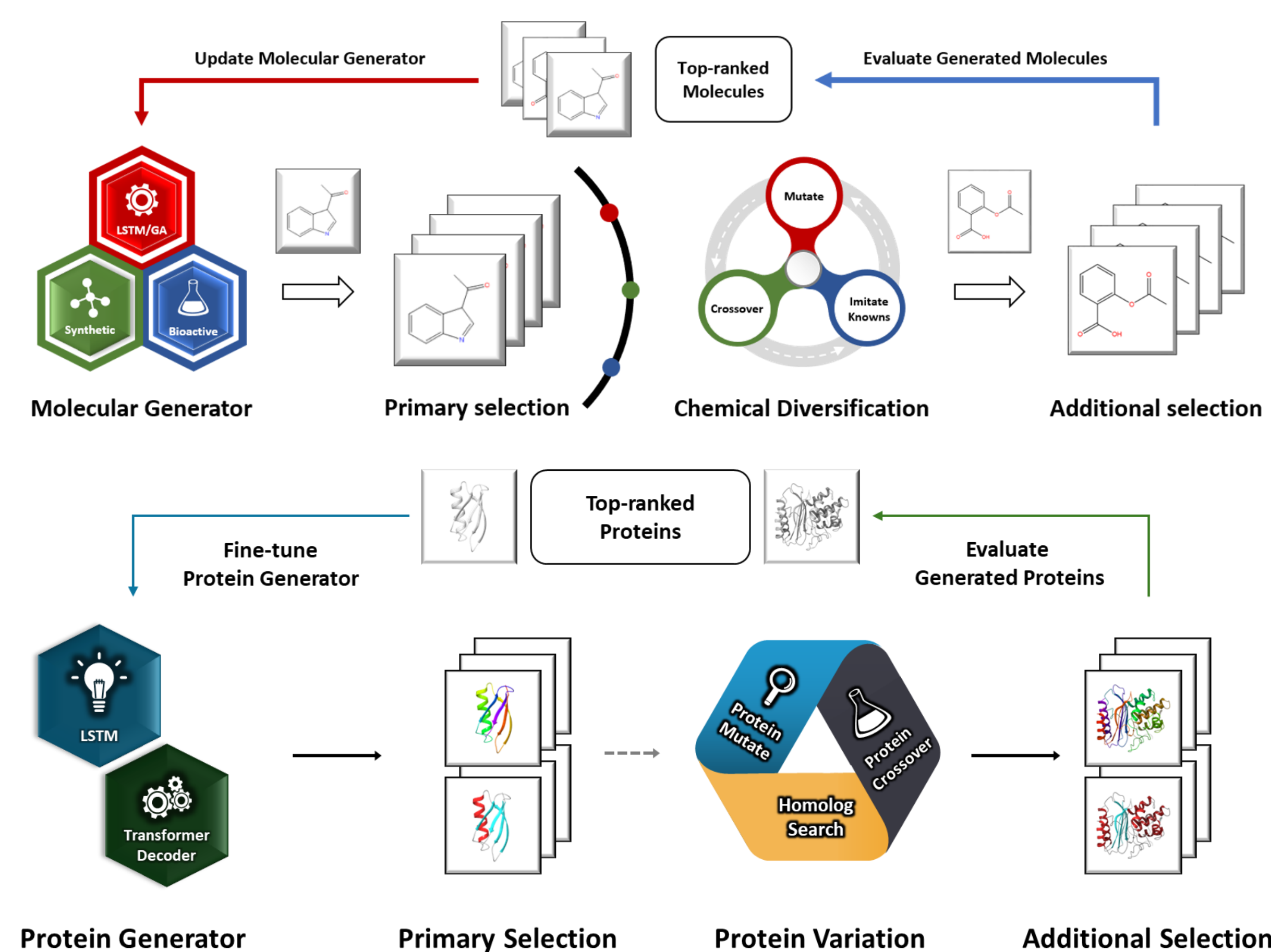
- 분자 생성 (Generative AI):**
딥러닝 분자 생성 모델을 활용한 신규 화학 구조 및 단백질 서열 공간 탐색
- 후보 선별 (QSAR & Screening):**
물성 및 표적 활성 예측 모델을 통한 가상 탐색 및 유효 물질 선별
- 정밀 검증 (Quantum Chemistry):**
전자 구조 계산 기반 머신러닝 위양성 정량 평가 및 분자 상호작용 검증
- 연산 확장 (Quantum Computing):**
양자컴퓨팅 알고리즘 기반 예측 정확도 향상과 대규모 연산 효율화 & 가속화

Multi-Objective Optimization in Vast Chemical & Protein Space

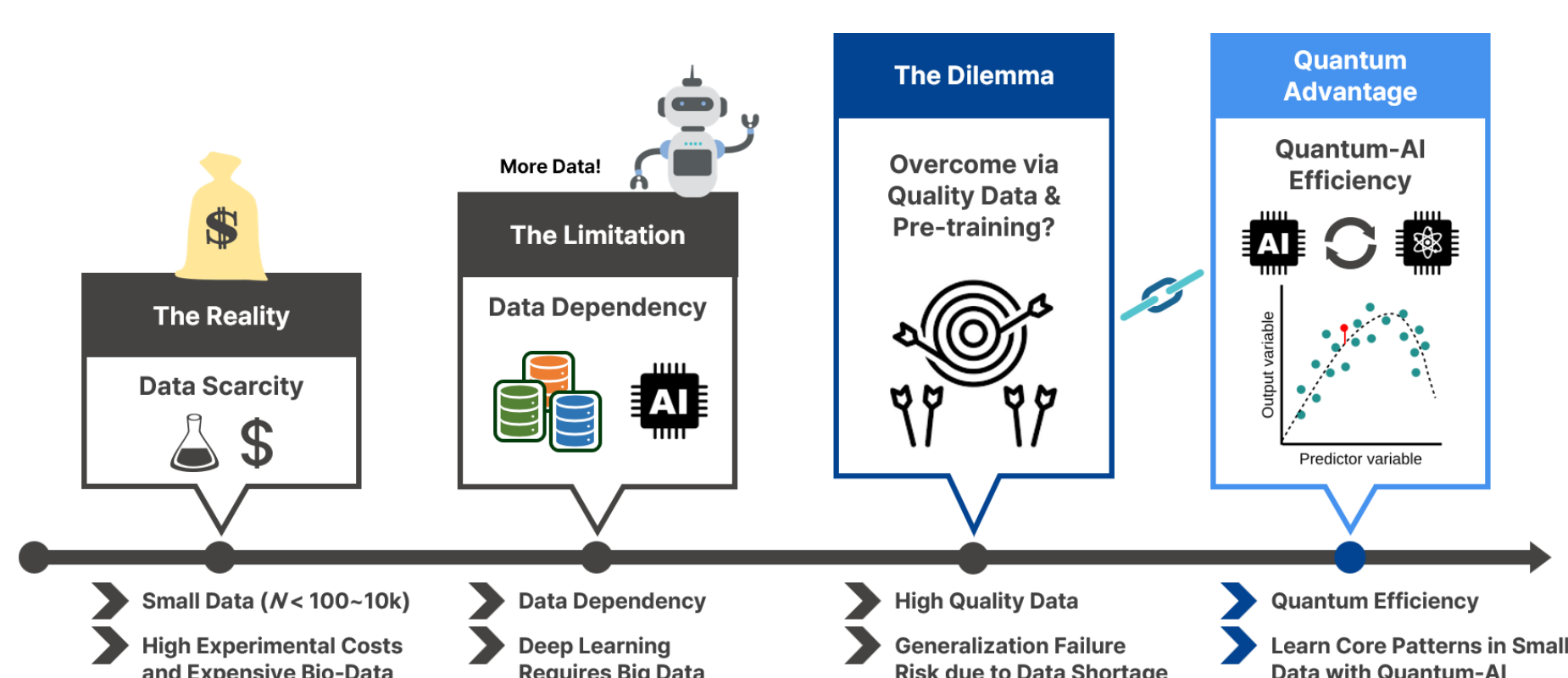
How can we efficiently explore vast chemical space to find new chemical entities?



Scoring-Assisted Generative Exploration (SAGE) for Molecular Design



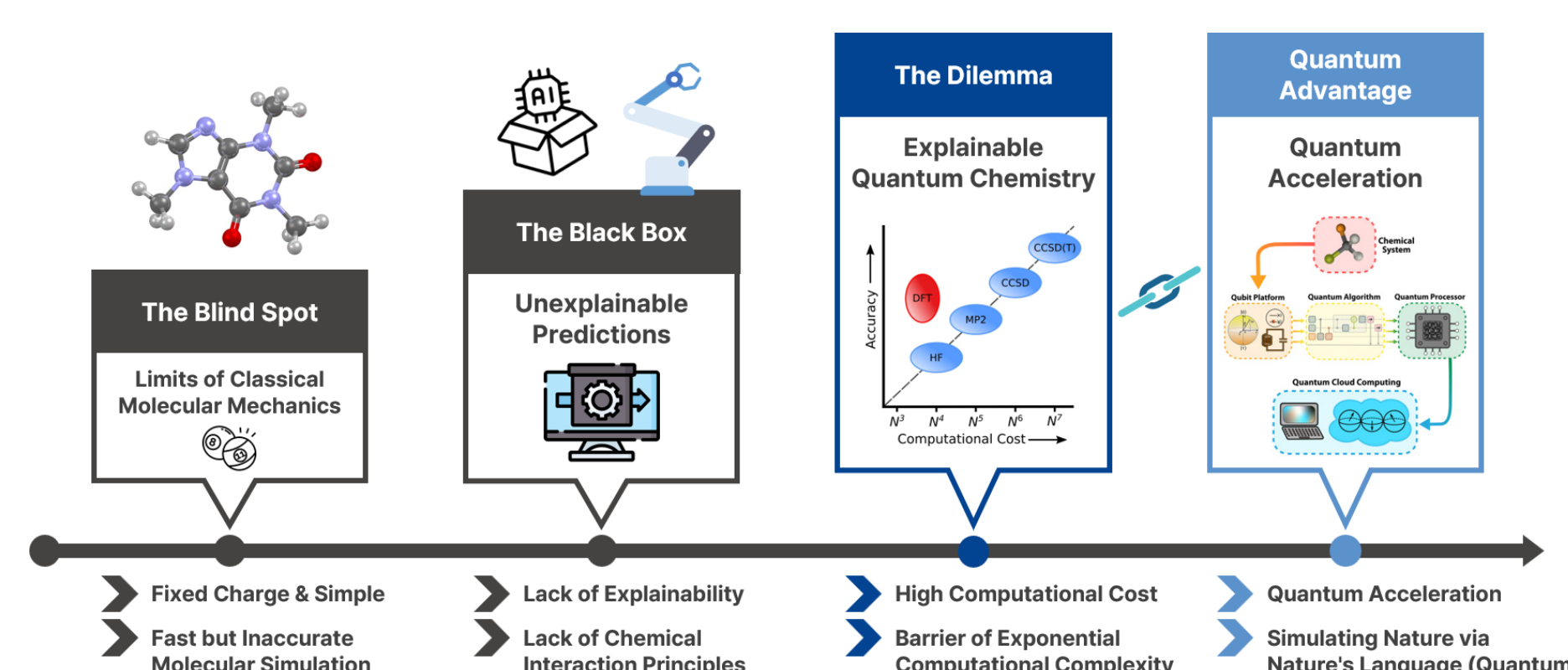
Quantitative Prediction



Quantitative Prediction for Rapid Screening

- Efficient Search of Vast Chemical Space:** High-speed search capability to capture key structures from chemical space.
- Guide Generative Models:** Provide accurate evolution direction for Generative AI via quantitative prediction.

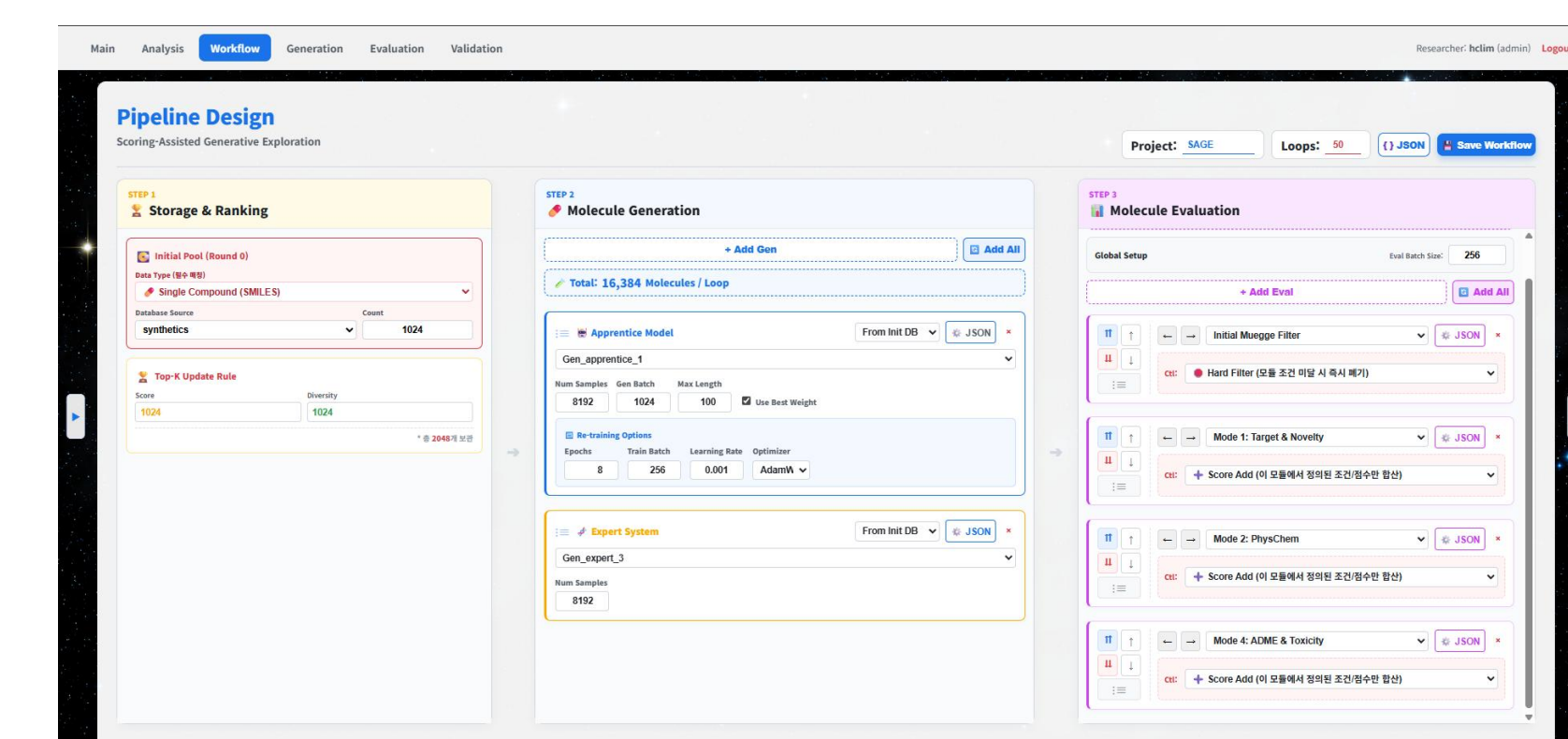
Molecular Simulation



Quantum Chemistry for Precise Validation

- Verify Physical Reality over Data Bias:** Validate actual natural effectiveness beyond AI's statistical patterns.
- Block False Positives & Secure Explainability:** Reveal physical causes of target-drug binding in quantum-level.

Q-SAGE Platform



Contact Information



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