Promethium

BOOST ADMET PREDICTIVITY WITH PROMETHIUM

ADVANCING DRUG DISCOVERY WITH GPU-ACCELERATED QUANTUM CHEMISTRY

TRANSFORM YOUR DRUG DISCOVERY PROCESS

Accurate prediction of absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties is essential for identifying promising clinical candidates early. Conventional machine learning approaches rely on hundreds to thousands of molecular features with millions of parameters, creating black-box models that can be easily prone to overfitting and limited generalization to novel scaffolds. Promethium's rapid quantum chemistry engine allows you to inject high-quality physics at an earlier stage of the pipeline, providing critical guardrails for AI. By combining density functional theory (DFT) quantum mechanical descriptors from Promethium with advanced machine learning approaches, high-accuracy ADMET predictions can be obtained that are both interpretable and trustworthy, essential for critical drug discovery decisions earlier in your optimization funnel

BREAKTHROUGH PERFORMANCE

Promethium-informed ADMET can help with Clinically Relevant Targets:

- **Caco-2 Permeability (Efflux):** Top 15 leaderboard ranking
- **BBB Classification:** 94% ROC-AUC exceeds published benchmarks
- **Intelligently curated quantum chemical features per molecule** vs. thousands of empirical features
- **Use up to 98% fewer model parameters** with superior predictive accuracy
- **Consistent DFT feature importance** across ADMET targets: Quantum properties validated as mechanistic drivers
- **Physics-based guardrails:** Predictions remain anchored in first-principles chemistry, reducing AI hallucination risk

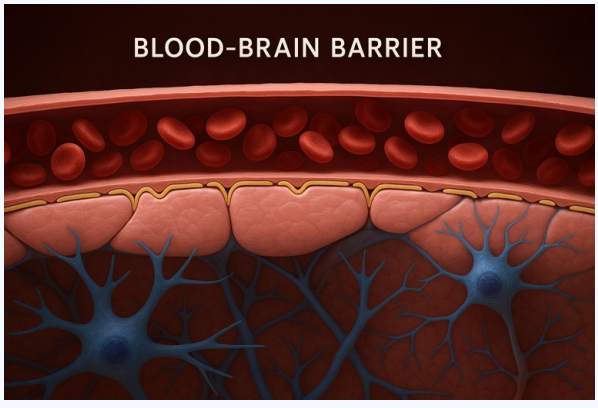
CASE STUDY: BBB

The Blood-brain barrier (BBB) is the lipid-rich membrane that controls access to the Central Nervous System (CNS). Drugs can cross the BBB via mechanisms such as passive diffusion, carrier-mediated transport and receptor-mediated transport. Molecular permeability across the BBB is influenced by factors such as the molecular size, lipophilicity, charge state and hydrogen bonding behavior. In this case study, quantum chemical descriptors such as the partition and hydration energies were calculated, as well as the polar surface area, and used to fit a BBB classification model based on datasets available in the literature.

METRIC	LITERATURE MODEL*	PROMETHIUM
Accuracy	86%	92%
Specificity	86%	93%
Recall	85%	91%
Precision	88%	93%
Model Size	>10^6 parameters	~10,000 parameters

*Faramarzi et al. 2022

Better accuracy with 98% fewer parameters!



Promethium is your physics-based partner for AI-driven drug discovery, providing the critically needed guardrails for artificial intelligence.
Promethium is trusted by leading pharmaceutical, therapeutics and biotech companies for accelerated, confident drug discovery.

WHY CHOOSE PROMETHIUM FOR ADMET?

CAPABILITY	TRADITIONAL APPROACH	PROMETHIUM (PHYSICS-BASED AI)
FEATURE ENGINEERING	Hundreds to thousands of empirical descriptors	Curated set of quantum mechanical + physical properties
INTERPRETABILITY	Black-box predictions, poor mechanistic link	Permutation importance sampling can identify quantum mechanical drivers
SET UP COMPLEXITY	Extensive parameterization required	Minimal configuration, fully automated
COMPUTATIONAL SPEED	Days to month of computation with conventional QM codes	Minutes for 1000s of candidates
GENERALIZATION	Limited to training chemical space, high failure rate on novel scaffolds	Physics-grounded transfer to novel chemotypes
ACCURACY	Variable across targets	Consistent R^2 signal and low MAEs
PARAMETER EFFICIENCY	$>10^6$ parameters prone to overfitting	>98% parameter reduction, robust predictions
AI GUARDRAILS	None, prone to hallucination and domain drift	Anchored in quantum mechanics and thermodynamics

KEY PLATFORM FEATURES

- **GPU-accelerated DFT:** 50-100x faster than incumbent toolsets
- **Parallel processing:** Score thousands of molecules simultaneously while maintaining physical rigor
- **100% physics-based features:** Quantum mechanical properties ensure transferability and mechanistic validity
- **Mechanistic insight:** Quantitative feature importance maps predictions back to underlying quantum properties
- **Guardrails against AI overfitting:** Physics-based feature space prevents spurious correlations and out-of-distribution failures
- **Seamless integration:** Promethium's Python SDK pairs effortlessly with scikit-learn, PyTorch, Chemeleon embeddings and other ML modalities
- **Cloud-native platform:** SaaS deployment; no hardware maintenance

DO MORE WITH PROMETHIUM

Beyond ADMET prediction, Promethium includes tools for comprehensive molecular design:

- **QC Score for Protein-Ligand Binding**
- **InteractionMap (F-SAPT) for Rational Ligand Design**
- **Chemical Reactions & Transition State Optimization**
- **Conformer Search and Torsion Scans**
- **Molecular Properties**

READY TO ACCELERATE YOUR DISCOVERY?

Apply quantum mechanical rigor to ADMET prediction at discovery timescales— without sacrificing accuracy or interpretability. Move beyond black-box empirical scoring to physics-grounded, trustworthy AI for critical candidate selection decisions.

READY TO LEARN MORE?

Get started today: Visit **promethium.qcware.com** for free trial access, technical documentation, and benchmark datasets.