Standigm®

AI for new drug R&D

QIP-ADMET

AI-Powered ADMET Predictor

Whitepaper | Paper | Try It Now | Demo Request

Accelerate Your Drug Discovery with Accurate QIP-ADMET

Experience how our Quantum-Informed Pretrained ADMET prediction models facilitate drug discovery with unparalleled accuracy and robustness. QIP-ADMET is trained on extensive datasets, including experimental data, in silico quantum mechanical (QM) data, and molecular descriptors, ensuring reliable performance and comprehensive ADMET insights.

QIP-ADMET: Standigm's AI-Powered ADMET Predictor

Harness the power of advanced AI to push the boundaries of pharmaceutical development and make data-driven decisions with confidence.

QIP-ADMET Key Features

⚙ **Exceptional Accuracy**

Rigorously validated with AUROC, AUPRC, and MAE metrics from the TDC ADMET dataset to ensure reliable performance.

⚙ **Comprehensive ADMET Insights**

Benefit from a wide range of predicted ADMET properties to guide your molecular optimization decisions.

⚙ **Advanced Molecular Understanding**

Leverage pre-training and shared representation framework to enrich molecular feature representations, providing deeper insights and overcoming the challenge of overfitting.

⚙ **Visual Explorations**

Easily visualize how changes in molecular fragments affect prediction scores with our intuitive, color-coded explanations.

Accurate ADMET Prediction with QIP-ADMET

Predictable ADMET Properties by QIP-ADMET

Absorption	BBB, logBB, Bioavailability, P-gp inhibition, P-gp substrate, Lipophilicity, Caco-2 permeability, water solubility, PBS kinetic solubility
Distribution	VDss (human), Microsomal clearance (human, mouse, rat), Hepatic clearance (human, rat), Protein plasma binding rate (human)
Metabolism	CYP substrate and inhibition (1A2, 2B6, 2C19, 2C8, 2C9, 2D6, 3A4)
Excretion	Liver microsomal stability (human, mouse, rat), Plasma stability (human)
Toxicity	DILI, Ames mutagenicity, Carcinogenicity (mouse, rat), Self-aggregation, hERG inhibition, Acute toxicity LD50

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Benchmark Comparisons
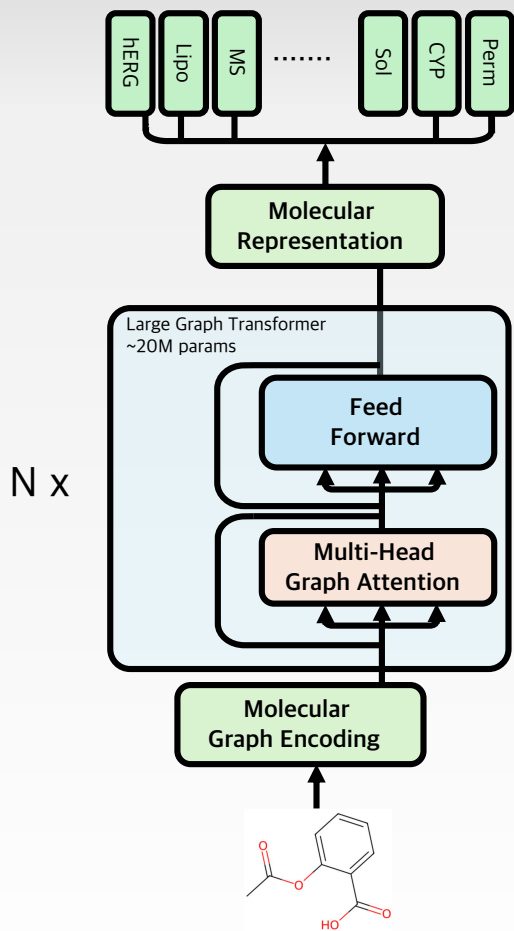
Benchmark comparisons with other commercial softwares (Predictor A, B, and C)

Experiment	Metric	Predictor A		Predictor B		Predictor C	Standigm QIP-ADMET
hERG inhibition	AUROC	Probability 0.636	hERG IC50 0.721	hERG pIC50 0.645		hERG 0.605	hERG **0.733**
Human microsomal stability	AUROC	Metabolic Stability 0.538		metabolism 0.528			MS-human **0.740**
Mouse microsomal stability	AUROC						MS-mouse **0.814**
Permeability (Caco-2)	AUROC	Caco-2 w/ logP 0.636	Caco-2 w/ logD 0.639	Caco-2 0.585	MDCK 0.570	Caco-2 **0.679**	Permeability 0.632
PBS kinetic solubility	AUROC	Solubility 0.814		PlogS 0.703	ClogS 0.767		Solubility-PBS **0.890**
Lipophilicity (logP)	MAE	logP 0.524					Lipophilicity **0.356**
CYP inhibition							
1A2	AUROC	0.772					**0.855**
2C9	AUROC	0.638					**0.779**
2C19	AUROC	0.663					**0.781**
2D6	AUROC	0.671					**0.782**
3A4	AUROC	0.700					**0.842**

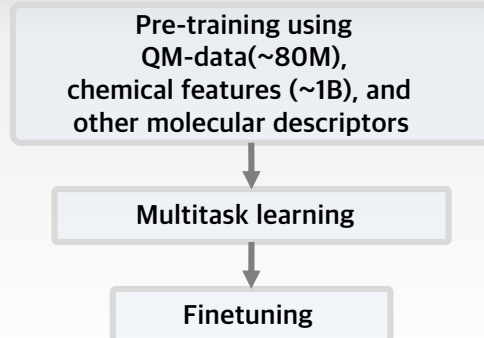Benchmark data are from PubChem/ChEMBL (CYP), Astrazeneca (Liphophilicity) and our in-house stocks (others)

QIP-ADMET Model Details

Model Architecture

Large Graph Transformer ~20M params

N x

- hERG
- Lipo
- MS
- ......
- Sol
- CYP
- Perm

Molecular Representation

Feed Forward

Multi-Head Graph Attention

Molecular Graph Encoding

Leveraging a transformer-based algorithm, our model significantly improves the representation of molecular structures.

Model Training

Pre-training using QM-data(~80M), chemical features (~1B), and other molecular descriptors

↓

Multitask learning

↓

Finetuning

Pretraining establishes a solid foundation, multitask learning expands versatility across diverse tasks, and finetuning sharpens specificity.

Enhancing Interpretation

Property A　　**Property B**

Property C　　**Property D**
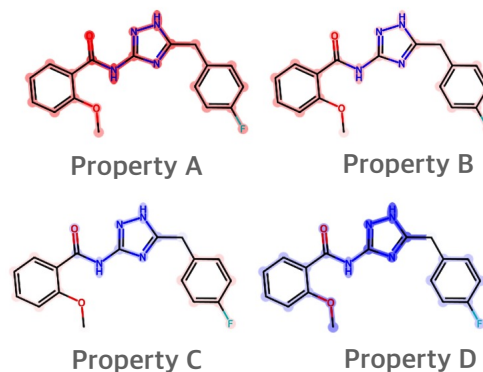
Enhancing interpretability in ADMET predictions by distinguishing between potentially improvable fragments (red) and degradable fragments (blue). This color-guided approach inspires chemists' intuition.

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