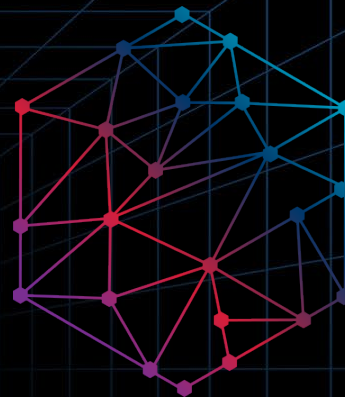


Model-Informed Drug Development

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# Introduction to ADMET Predictor®

David Miller

# ADMET Predictor Overview

## Property Prediction

Physicochemical  
Metabolism  
Transporters  
Toxicity  
ADMET Risk

## PBPK Simulations

%Fa, %Fb  
Cmax, Tmax, AUC, T<sub>1/2</sub>, CL  
Cp-time curves  
Optimal dose

## Model Building

Activity, properties  
Molecular + atomic descriptors  
Regression, classification  
Uncertainty, confidence

## Cheminformatics

Compound design  
Scaffold clustering  
R group analysis  
Similarity / diversity



# ADMET Predictor Deployment

```

david@LAPTOP-41G2D2G8 ~
$ ADMET_Predictor.exe -t SDF -m SIMFaFb Data.sdf
    
```

Command line

**GastroPlus®**

Input Structure Properties

Selected Compound: Molecule 1

Simulation Parameters:

- Time: 0 to 1000
- Time Step: 10
- Time Step (min): 10
- Time Step (max): 1000
- Time Step (avg): 100
- Time Step (std): 100
- Time Step (min): 10
- Time Step (max): 1000
- Time Step (avg): 100
- Time Step (std): 100

Effective Permeability

Score: 5.52

ADMET Metrics:

- ADMET Score: 1.15E+17
- ADMET Score: -11.953
- ADMET Score: 2.82E+14

KNIME Analytics Platform

ADMET Predictor v8.5

Table View - 036 - Interactive Table (ADMET Predictor Output)

Row ID	mol	Molecular Weight	QED	TPSA	TPSA5	TPSA6	TPSA7	TPSA8	TPSA9	TPSA10	TPSA11	TPSA12	TPSA13	TPSA14	TPSA15	TPSA16	TPSA17	TPSA18	TPSA19	TPSA20	
Row0		1	4.75	0.74	0.28	0.77	2.45	0.84	1.64	1.52											
Row1		2	1.04	1.254	-0.011																
Row2		3	0.68	1.589	1.309																
Row3		4	1.124	1.06	0.502																
Row4		5																			
Row5		6																			

KNIME / Pipeline Pilot

ADMET Predictor Desktop

Structure

Star Plot

ADMET\_Risk: 0.000, 2.405, 0.011

ADMET\_Code

Unselected (229)

Selected (71)

Plasma Concentration - CIMETIDINE

Concentration (ng/ml) vs Time (h)

Species: human

Route: IV tablet

Dose: 100 mg

Time: 0-100 h

Cratic: 2.67 ng/ml/h

Time: 2.5 h

AUC: 9.47 ng/ml/h

AUC(0-100 h): 94.7 ng/ml

CL: 41.66 L/h

Desktop

# ADMET Predictor Feature Tour

- Key Takeaways
  - Functionality spans early discovery through preclinical
  - Ultrafast calculations and flexible license policy means a single license allows simultaneous use by an entire organization



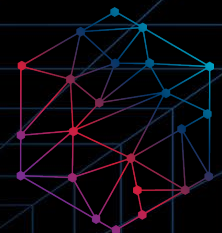
# Q & A

Questions & Answers

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