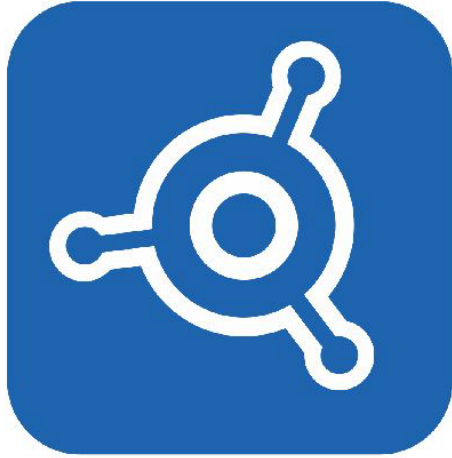


Ex-Lilly Luminaries

Ground Truth: How the
Data Fuels What AI Can
Do in Drug Discovery



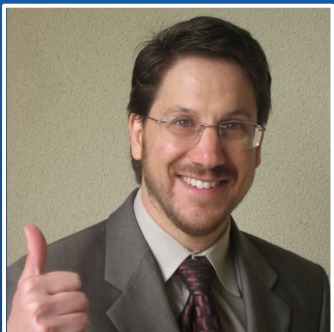
**CDD Vault
Webinars**



CDD VAULT[®]
Complexity Simplified



Lilly
TuneLab[™]



Barry Bunin, PhD

- CEO & Board Director, Collaborative Drug Discovery



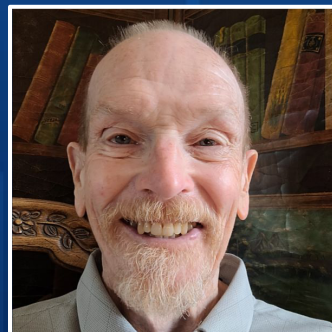
Mic Lajiness, MS

- Independent Consultant
- Former Research Advisor, Eli Lilly & Company



Aliza Apple, PhD

- VP Catalyze360 AI/ML & Global Head of Lilly TuneLab at Eli Lilly & Company



Jim Wikel, MS

- Chief Chemistry Officer, Apex Therapeutics
- Former Head of Computational Chemistry & Structural Biology, Eli Lilly & Company



Mary Mader, PhD

- President, MM Molecular Pharma Consulting
- Former Research Fellow, Eli Lilly & Company

#1

**Can you describe how
informatics works in a big
pharma vs. smaller
biotechs?**

#2

**How, philosophically, might
one get the best of both
worlds?**

#3

What were the key concepts you learned working in drug discovery? What learnings do you think would save others time?

#4

**What are the challenges
communicating between
biologists and chemists?**

#5

**What are the challenges
communicating between
computational
informaticians and
experimentalists?**

#6

**What do you think of Lilly
TuneLab and CDD Vault?**



Example of TuneLab Predictions

TuneLab Predictions ?

[Edit](#)

ADME ?

Permeability Papp, MDCK, AB

0.884 (0.143-0.764) 10^{-6} cm/sec

Intrinsic Clearance

Species	Hepatocytes (μ L/min/million cells)	Liver Microsomes (μ L/min/mg)
Dog	0.231 (0.237-0.876)	
Human	0.962 (0.320-0.504)	0.986 (0.271-0.925)
Mouse	0.354 (0.397-0.827)	0.629 (0.123-0.633)
Rat	0.311 (0.235-0.610)	0.950 (0.137-0.757)

Fraction Unbound

Species	Brain	Liver Microsomes	Plasma
Human	0.398 (0.276-0.776)	0.274 (0.360-0.577)	0.0817 (0.106-0.634)
Monkey			0.0952 (0.158-0.617)
Rat			0.673 (0.0346-0.689)

Physchem ?

Kinetic Solubility

pH 2.0	< 0.01 mg/mL	< 0.1 mg/mL
pH 6.0	$\geq$ 0.01 mg/mL	< 0.1 mg/mL
pH 7.4	$\geq$ 0.01 mg/mL	$\geq$ 0.1 mg/mL

Tox ?

hERG Binding, Astemizole, IC50

< 10 μ M (uncertain)

Phospholipidosis, HepG2

lysosomotropic

Primary Hepatocyte Cytotoxicity, Rat, LC50

non-lethal ($LC_{50} > 100 \mu$ M)

Metabolic Stability

Species	% parent loss	> 60% turnover
Dog		not extensively metabolized (< 60% turnover)
Human	0.968 (0.388-0.777)	extensively metabolized (> 60% turnover)
Monkey		extensively metabolized (> 60% turnover)
Mouse	0.0752 (0.0614-0.739)	not extensively metabolized (< 60% turnover)
Rat	0.890 (0.284-0.886)	not extensively metabolized (< 60% turnover)

CYP Inhibition

2C9	< 50%
2D6	> 50%
3A4	> 50%

Select individual models or saved sets

Select model endpoints

?

Saved sets

+

Project ABC

2 models

+ - ✎ 🗑

Project DEF

9 models

+ - ✎ 🗑

Filter models by name or version...

Select [all](#) / [none](#)

^ ☒ CYP Inhibition 1/3

☒ Human, 2C9, 10 μ M, % inhibition; 50 Cls

The model predicts if a compound at 10uM shows >50% or <50% CYP2C9 inhibition in human hepatic microsomes. (version: 2025-06)

☐ Human, 2D6, 10 μ M, % inhibition; 50 Cls

The model predicts if a compound at 10uM shows >50% or <50% CYP2D6 inhibition in human hepatic microsomes. (version: 2025-06)

☐ Human, 3A4, 10 μ M, % inhibition; 50 Cls

The model predicts if a compound at 10uM shows >50% or <50% CYP3A4 inhibition in human hepatic microsomes. (version: 2025-06)

^ ☒ hERG Binding 1/1

☒ Astemizole, IC50, μ M; <10,>30 Cls

This model predicts hERG astemizole binding IC50 class (<10 uM or >30 uM). hERG is a voltage gated potassium channel involved in cardiac repolarization. Off target hERG inhibition could indicate cardiac toxicity. (version: 2025-06)

^ ☐ Fraction Unbound 0/5

^ ☐ Intrinsic Clearance 0/7

2 Models selected

Astemizole, IC50, μ M; <10,>30 (Classification) ✕

Human, 2C9, 10 μ M, % inhibition; 50 (Classification) ✕

Cancel

Predict

Questions?

Learn more:

collaborativedrug.com

Free personalized demo & trial:

info@collaborativedrug.com

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