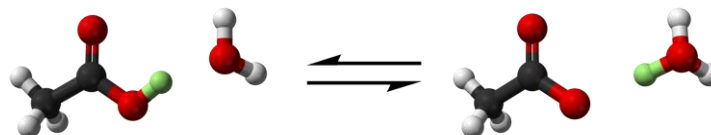# Cheminformatics Predictions

PSCI-518,Spring 2024
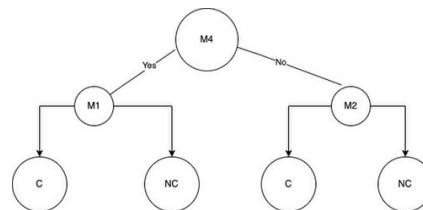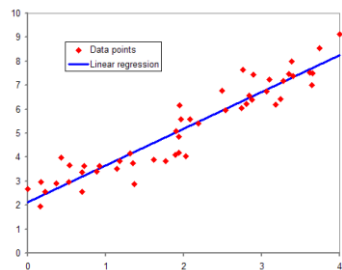
Noam Morningstar-Kywi

Types of Predictive Models

- Deterministic/Calculated

- Empirical

- Machine Learning (Decision Trees, Neural Networks , etc.)
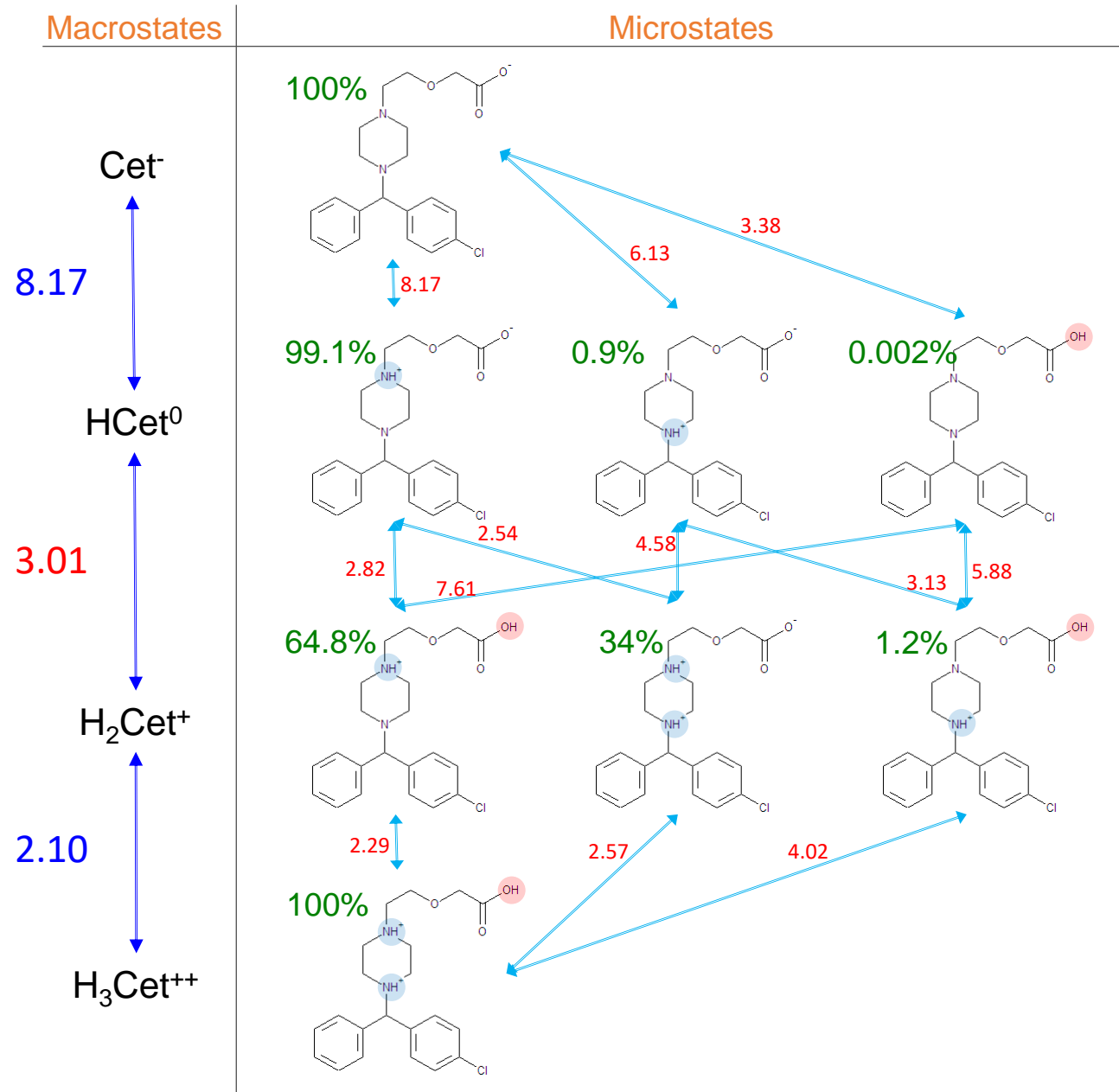
- Theoretical/Mechanistic

- Trains

Example: pKa Prediction

Need to predict two things:

- Ionizable groups
  - Protonation vs deprotonation
- Dissociation constants
  - Numerical value

Different approach used for each

Then need to calculate and classify macroconstants ("traditional" pKa)

Experimental Data

- What can be detected?

- What is the limit of detection/quantification?

- What is the sensitivity/confidence of the assay?

- What is the error range between replicates?

		Papp A→B (cm e-6/s)	Papp B→A (cm e-6/s)	Efflux Ratio
Replicate 1	Compound	<0.1	<0.1	
	Compound + zosuquidar	<0.1	<0.1	
Replicate 2	Compound	0.11	0.15	1.4
	Compound + zosuquidar	0.13	<0.1	

GastroPlus Activities

- Create "experimental" record, add pKa & LogP

- Compare results to pure ADMET Predictor predictions

- Put in observed Cp-time data (.ipd), setup IV dose, compare results