# ADMET Prediction



Brain

A

D

M

E

Liver

Kidney

| Absorption |
|---|
| Caco-2, LogP |

| Distribution |
|---|
| Vd, PPB |

| Metabolism |
|---|
| CYP450 |

| Excretion |
|---|
| Clearance |

| Toxicity |
|---|
| hERG, LD50 |

## Pharmacokinetic Profile



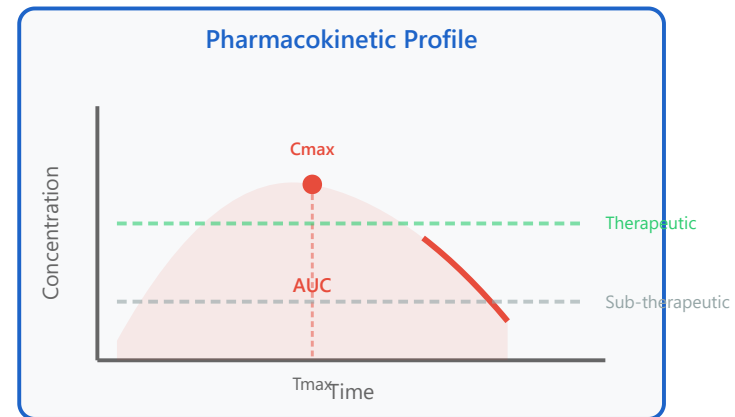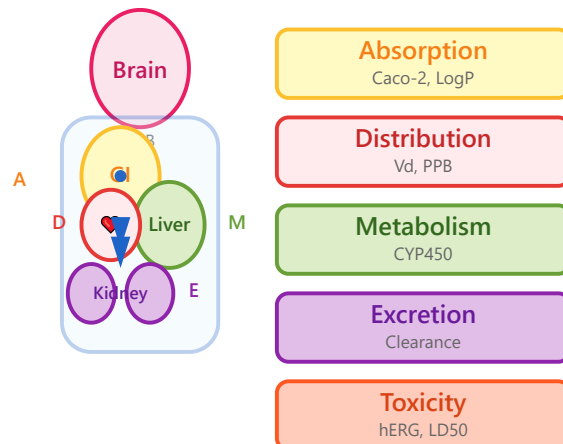Concentration

Cmax

Therapeutic

AUC

Sub-therapeutic

Tmax Time

### Absorption models
Oral bioavailability prediction

### Distribution (BBB, Vd)
Tissue distribution modeling

### Metabolism (CYP)
Drug metabolism prediction

### Excretion (clearance)
Elimination pathway modeling

### Toxicity endpoints
Safety assessment