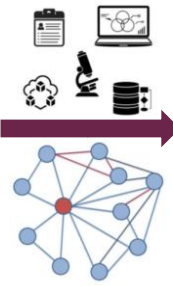
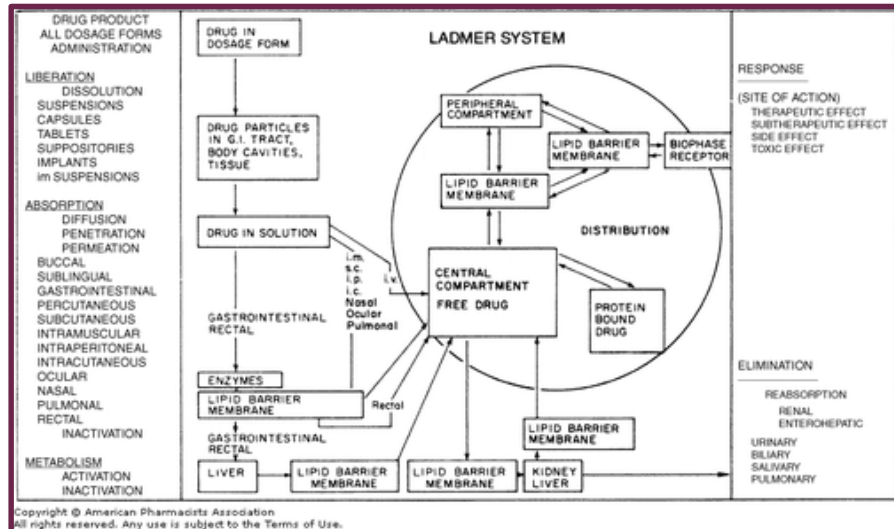
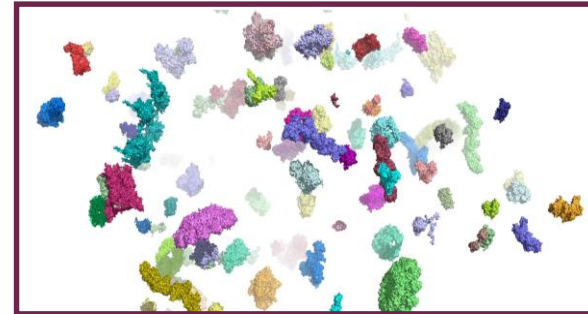


ADME-TOX IN 3D, DL & CHEMINFORMATICS

The LADMER system [Liberation, Absorption, Distribution, Metabolism, Elimination, Response]

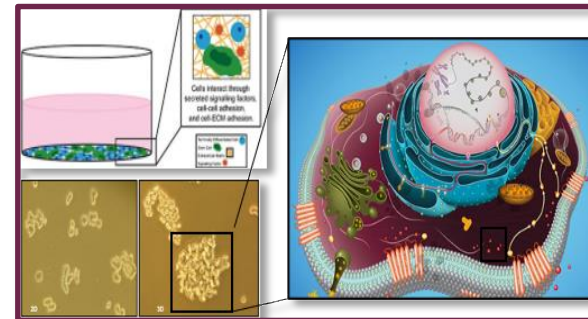


In silico ADME-Tox assays



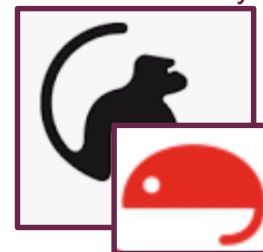
- 3D-QSAR [Quantum Structure-Activity Relationship] models
- Molecular docking
- Molecular dynamics
 - Quantum mechanical methods
 - Molecular mechanical methods
- Pharmacophore modelling

In vitro ADME-Tox assays (3D models)



- 3D cell metabolism studies
- Live cell studies
- CYPs inhibition studies
- CYPs induction studies
- Protein binding studies
- RBC partitioning studies
- Permeability studies
- hERG studies
- Mechanistic toxicity/ cytotoxicity studies

In vivo ADME-Tox assays (animal studies)



- DMPK [Drug Metabolism Pharmacokinetic] studies
- Toxicokinetic studies