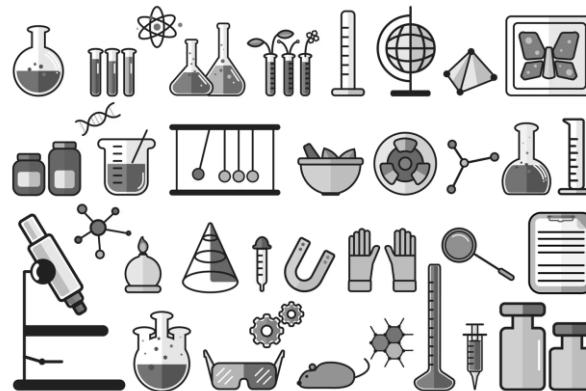# ADME-TOX IN 3D, DL & CHEMINFORMATICS

In silico ADME-Tox

- 3D-QSAR models
- Molecular docking
- Molecular dynamics
- Quantum mechanical methods
- Molecular mechanical methods
- Pharmacophore modelling

In vitro ADME-Tox

- 3D cell metabolism studies
- Live cell studies
- CYP450 studies
- Protein binding studies
- RBC partitioning studies
- Permeability studies
- hERG studies
- Mechanistic toxicity/ cytotoxicity studies

In vivo ADME-Tox
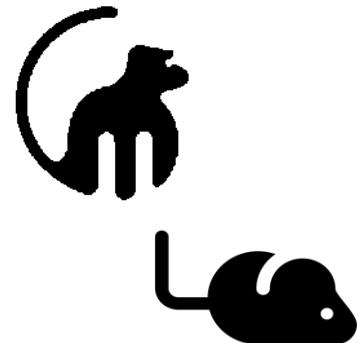
- DMPK studies
- Toxicokinetic studies