

Solution and Pharmaceutical Chemistry of (Metallo)drugs
(KDIT105)
thematics

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Basic definitions of pharmaceutical/medicinal chemistry.

Classification of drugs. Introduction to pharmacodynamics and pharmacokinetics.

Therapeutic index; side effects; drug development steps; clinical trials.

Prodrug concept (metallic, nonmetallic)

Factors affecting pharmacokinetics (LADME properties: liberation, absorption, distribution, metabolism, excretion), bioavailability, accumulation, biofluids; routes of drug administration.

Acid-base properties: macroconstants and microscopic proton dissociation constants; lipophilicity, solubility and their modifications.

Experimental determination of pK_a and $\log P$ values. Biological pH-buffers.

Metal containing drugs (various biological activities; chelate therapy).

Solution stability of metal complexes, complex formation equilibrium processes; conditional stability constants; computation of concentration distribution curves.

Experimental determination of stability constants (pH-potentiometry, UV-visible spectrophotometry, CD spectroscopy, fluorimetry, NMR and EPR); lipophilicity of metal complexes; redox properties of metal complexes (cyclic voltammetry, UV-visible spectroelectrochemistry).

Effect of interaction with biological macromolecules (proteins, DNA) on pharmacokinetics; plasma protein binding; experimental determination of binding sites and binding constants of protein-ligand adducts (spectroscopic and separation methods)