

### Medicinal chemistry

Definition:

**Drugs:** A medicine or other substances which has a marked effect when taken into body.

**Medicine:** A drug or other preparation is taken into body in order to treat or prevent disease

**Drug Name:** Adopted by company during development

**Proprietary Name:** Registered & used by company exclusively

**Systemic Name:** By IUPAC rules

**Research Code:** Letter & no. For company to identify the particular compound

**Generic Name:** Recommended international non proprietary name by WHO when patent has expired

Classifications of drug

**Chemical Structure:**

Common skeleton structure

May have same biological activity

**Pharmacological effect:**

Same biological outcome, different pathway

Limit drug use eg. :anti-fungal

**Target System:**

Same biological outcome different pathway(Specific chemical messengers)

Synthesis,mimics,blocks,degradation

**Target Molecule:**

Affects specific enzyme, neurotransmitter or receptors

Same biological outcome, same pathways

Similar structure

Membrane Permeability coefficient :

1. Depend on lipophilicity & molecular charge
2. Large coefficient = Good permeability ; Small coefficient = Poor permeability- highly charged (+/-)
3. ~80% drug posses a charge, depend on pH of the medium & pKa of a FG

### pKa

**Bronsted-Lowry Theory**



Acid + Base  $\rightleftharpoons$  Conjugated Base + Conjugated acid

**Henderson-Hasselbalch**

$pKa = pH - \log\left(\frac{[Conjugated\ base]}{[Weak\ acid]}\right)$

**pKa:** pH at which 50% of substance is ionized

### pKa (copy)

**Bronsted-Lowry Theory**



Acid + Base  $\rightleftharpoons$  Conjugated Base + Conjugated acid

**Henderson-Hasselbalch**



### pKa (copy) (cont)

$pKa = pH - \log \left( \frac{[\text{Conjugated base}]}{[\text{Weak acid}]} \right)$

**pKa:** pH at which 50% of substance is ionized

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