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

$HA + B \rightleftharpoons A^- + HB^+$
Acid + Base ⇌ Conjugated Base + Conjugated acid

Henderson-Hasselbalch

pKa = pH- Log([Conjugated base]/[Weak acid])
pKa: pH at which 50% of substance is ionized

pKa (copy)

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pKa (copy) (cont)

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