Pharmacorner

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Contact : Pharmacorner2011@gmail.com

- BCG - Vaccine Lab. → Madras / Chennai
- Central Drug Testing Lab (CDTL) → Bombay
- Central Drug Laboratory (CDL) → Calcutta → Biological & microbiological
- Central Drug Research Institute (CDRI) → Lucknow
- Central Research Institute (CRI) → Kasauli → Sera, Antitoxin, Antigen, Vaccine
- Indian Drug Mfrs. Association (IDMA) → Bombay
- Indian Society of Blood Transfusion & Immunohaematology → Pune
- Indian Veterinary Research Institute - I33atnagar
- Central Indian Pharmacopoeia Laboratory (CIPL) - Ghaziabad → (Condoms)
- National Plasma Fraction Centre - Bombay
- National Institute of Communicable Disease - New Delhi → Polio Vaccine
- National Institute of Virology - Pune
- Organisation of P'cal Producers - (OPPI) - Bombay
- Dabur Research Foundation - Ghaziabad.
- Ministry of Defence - Kanpur
- WHO - Geneva.
- BP. Commission - London
- AIIMS - New Delhi
- Tata Memorial Hospital - Bombay
- Kothari Medical Centre → Calcutta.
- University College of Medical Sciences & Guru Teg Bahadur Hospital → Delhi

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Delhi → National Institute of Communicable Disease → Applied
→ AIIMS → Guru Teg Bahadur Hospital → Inst. of Manpower Research

Bombay → CD Testing Lab. → IDMA → National Plasma Fract. Centre
→ Org. of P'cal Producers (OPPI) → Tata Memorial Hospital

Madras → BCG-Vaccine Lab.

Calcutta → CDLab., Kothari Medical Centre

National P'cal Pricing Authority (NPPA) - Aug - 1997

Lucknow → CDRI // Kasauli → CRI

Ghaziabad → Central Indian P'copeia Lab., Dabur

Pune → Indian Soci. of Blood Transfusion & Immunohaematology
National Insti. of Virology

I33atnagar → Indian Veterinary Research Institute

Kanpur → Ministry of Defence
→ Synthetic Drug Plant → Hyderabad (IDPL) / IP - 1946 from BP - 1932.

* Jury :-

Poison Act → 1919 // Opium Act - 1857, 1878

Dangerous Drug Act - 1930 — Cruelty To Animal Act - 1960, Insecticide Act - 1968

Drug Act - 1940 , Drug rules - 1945

Pharmacy Act - 1948

Advisory Board - DTAB (Drug Technical Advisory Board) & DCC (Drug Consultative Committee)

Preconstitution → Opium Act - 1857, 1878 // Poison Act - 1919
Dangerous Drug Act - 1930 // Drug Act - 1940.

Post-constitution → Pharmacy Act - 1948, Drug & Magic Remedies (Objectionable Advertisement) - 1954

- Medicinal & Toilet Prep^n (Excise Duties) - 1955, 1976 → Ethanol
- The Drugs (Price Display & Control) Order - 1966 - 70 - 69 87 95
  ↳ 1962 - revised
- Insecticides Act - 1968
- Medical Termination of Pregnancy Act - 1971 - 75 (Act / Rules) EXCISE
- Narcotic Drugs & Psychotropic Subs. Act - 1985

* Drug & Cosmetic Act - 1940

→ Drug Policy - 1986. / Patent Act - 1970 - 72 - 99

PCI → Elected - Six ⇒ UGC - (Pharmacy, P. chem., cogno., cology)
↳ 1 - MCI, 1 - State Council.
↳ Nominated - Six ⇒ UGC representative & AICTE (1987)
↳ Ex-officio ⇒ Director General of Health Services, ⟺ State Govt.
Director - CDL, Drug Controller of India

* Cosmetic Colour → 2 ppm - Arsenic, 20 ppm - Lead
100 ppm - Heavy Metal.

* Schedule - G → Cancer, Diuretic, Oral hypoglycaemic, Hydantoin, Insulin, Antihistaminic

* Schedule - O → Grade - 1 (18), 2 (10), 3 (05)

* Sch - F → Vaccines, Toxins, Antigens & Sera.

* Sch - W → Generic Names → Analgin, FeSO4, Aspirins, Piperazines, Chlorpromazine

* Sch - M & U → 1988

QSAR

Corwin Hansch → 1964 → SAR in Quantitative terms.
→ Crum-Brown & Fraser → 1868 → Curare → 4°-$NH_4^\oplus$
→ Richardson → Aliphatic alcohol → mol. wt. → Hypnotic.
→ Meyer & Overton → Insecticidal → Boiling point
→ Narcotic → Surface Tension. (Kolw)

* QSAR - Methods:- (I) Free-Energy Models.
(a) Hansch method - Linear Free Energy relationship
(b) Martin & Kubinyi - non-Linear
(c) Free-Wilson Mathematical model.
(II) Other Statistical Methods :-
(a) Discriminant Analysis → Yvonne Martin - 1974 (1 or 0)
(b) Principal Component Analysis
(c) Factor Analysis
(d) Cluster Analysis → $P < 0.05$
(e) Combined Multivariate Analysis
(III) Pattern Recognition
(IV) Topological Method → Steric misfit & receptor (MTD)
(V) Quantum Mechanical Method
(VI) Molecular Modelling

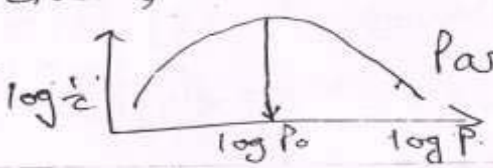
* Increase in Entropy Leads to stabilization of drug-receptor complex. ∝ to nonpolar part of drug's surface Area.

* 1-octanol ⇒ 1.7 M water ⇒ Low Vapour Pressure
↳ UV-transparent.

⇒ Negative π-value → prefer aqueous phase
Positive π-value → prefer Organic phase

⇒ $\log \frac{1}{C} = a \log P + b$ [Linear Relationship]
↳ Activity ↑ as & ↑ in lipophillicity
eg:- protein binding drugs, unspecific toxic, anaesthetic, bactericidal, fungicidal, narcotic, hemolytic, phenyl ethylamines

⇒ Non-Linear



$R_m = \log\left(\frac{1}{R_f} - 1\right)$ → Not true equilibrium parameter

Ortho effect → o-disubstituted leads to low log P & π-value

$\Delta\pi$-ortho = (π O-subst) − (π P-subst.)

MV. $\frac{\text{mol. wt.}}{\text{density}}$

MR (Refractivity → volume + sum of electron polarisability) $= \frac{n^2-1}{n^2+2} \cdot \frac{\text{mol. wt.}}{\text{density}}$ → measure of dispersion forces (dipole-induced dipole forces)

$\Rightarrow PA = R^{\frac{1}{4}} \frac{\text{mol. wt.}}{\text{density}}$

MR & Parachor are corrected Molar Volumes

Lipophilicity Factor by HPLC $= k' = \frac{t_R - t_0}{t_0}$

Fragmental f constant $\Rightarrow$ π-value.

Electronic Parameter

- Hammett Constant → HC Brown constant (σ_p) (benzoic a, anilines, phenols → dimethylphenyl-carbinyl chlorides)
- Polar effect (σ_I) → Mesomeric effect (σ_R)
- Taft's polar substituent constant (σ^*) ⇒ aliphatic ester hydrolysis
- Homolytic Constant (⇒ free-radicals)
- Field & Resonance component (F & R) ($\sigma_m \pm \sigma_p$)

$P = \frac{(n^2-1)M}{(n^2+2)d}$ ← Lorenz-Lorenz

$\log k = 4.2 - 1.00 \Sigma\sigma$ ← Hammett eqn.

Where Negative σ ⇒ e^--releasing nature of substituent

Taft's Constant $= E_s = \log(k/k_0)$

CH_3 = Zero (⇒ Intramolecular steric effects)

MR, van der Waals radii, mol. wt.

Molecular connectivity index (χ) (indicate degree of branching)

(molecular substructures in Topological terms)

→ lipophilicity & Steric features.

→ e^- withdrawing inductive effect ⇒ use-H bonding

⇒ ↑ lipophilicity ⇒ ↑ log P & π-values.

Gaussian eqn → Rate of drug act^n = A = f(log P) = $a \cdot \exp\left[-(\log P - \log P_0)^2 / b\right]$

≠ → Hansch model ⇒ $\log \frac{1}{c} = K_1\pi + K_2\sigma + K_3 E_s + K$

→ Free-Wilson ⇒ $\log \frac{1}{c} = \mu + \sum a_{ij}$

→ Mixed (Kubinyi) ⇒ $\log \frac{1}{c} = \sum a_{ij} + \sum K_j \phi_j + K$

* $(+\pi)$ & $(-\sigma)$ ⇒ e^- releasing groups

$(-\pi)$ & $(+\sigma)$ ⇒ e^- withdrawing groups

* Topliss Approach ⇒ Also Craig plot, Fibonacci search method & Sequential Simplex Strategy.

* Craig plot

$(+\sigma, -\pi)$	$(+\sigma, +\pi)$
SO_2NH_2, $CONH_2$, $COOH$	NO_2, CF_3, F
NH_2, CH	C_2H_5, CH_3, C_4H_9
$(-\sigma, -\pi)$	$(-\sigma, +\pi)$

* Bonding Interactions — Stretching, Bending & Torsional (NMR)
  - Equilibrium Type (Bond angle, length) ↳ X-ray, neutron or e^- diffraction
  - Force constant Type → UV-vis or IR ↳ Stretching or bending force constant

* Non-Bonding Interact^n:-
- Dispersive attract^n (vander Waal), - dipole-dipole interact^n.
- Charge-charge interact^n ⇒ London, Coulomb.

* Molecular Dynamics
  - Monte Carlo method ⟶ $X = \frac{\sum_i X_i \exp(-E_i/KT)}{\sum_i \exp(-E_i/KT)}$
  - Molecular dynamic method.

* Quantum Mechanics:-
  - Schrodinger Eq^n method - Extended Huckel method
  - Complete Neglect of Differential Overlap (CNDO)
  - Intermediate Neglect (INDO)
  - Modified Intermediate (MINDO)
  - Neglect of Diatomic Differential Overlap (NDDO)
  - Modified NDDO (MNDO)

* CoMFA (Comparative Molecular Field Analysis) → 3D
* Simulated Annealing * Neural Networks
* Contour Plots (CoMFA) * Pharmacophore Mapping (↔ Dock)
* MSA - Molecular Shape Analysis (↔ Common Overlap Steric Volume - COSV)

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