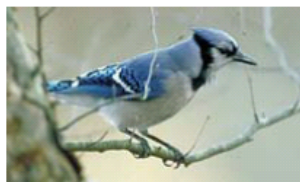


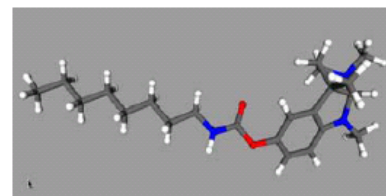
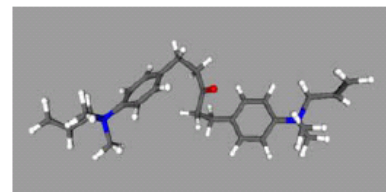
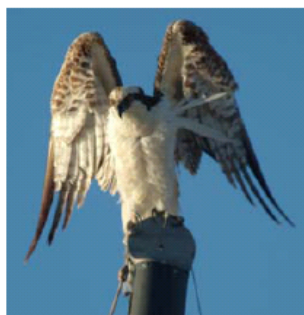
QSAR

BT 305

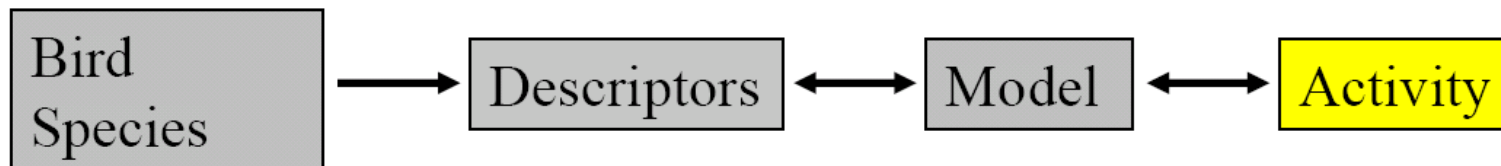
QSAR (of birds):



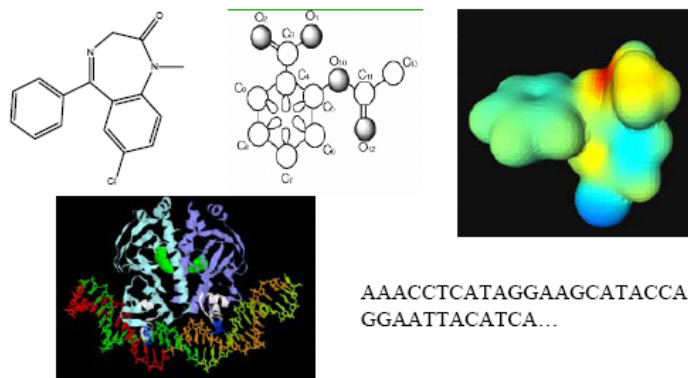
QBSPR: What is flight performance? Performance = muscle efficiency * flight time as
($P = \text{Efficiency} * \text{Time}$)



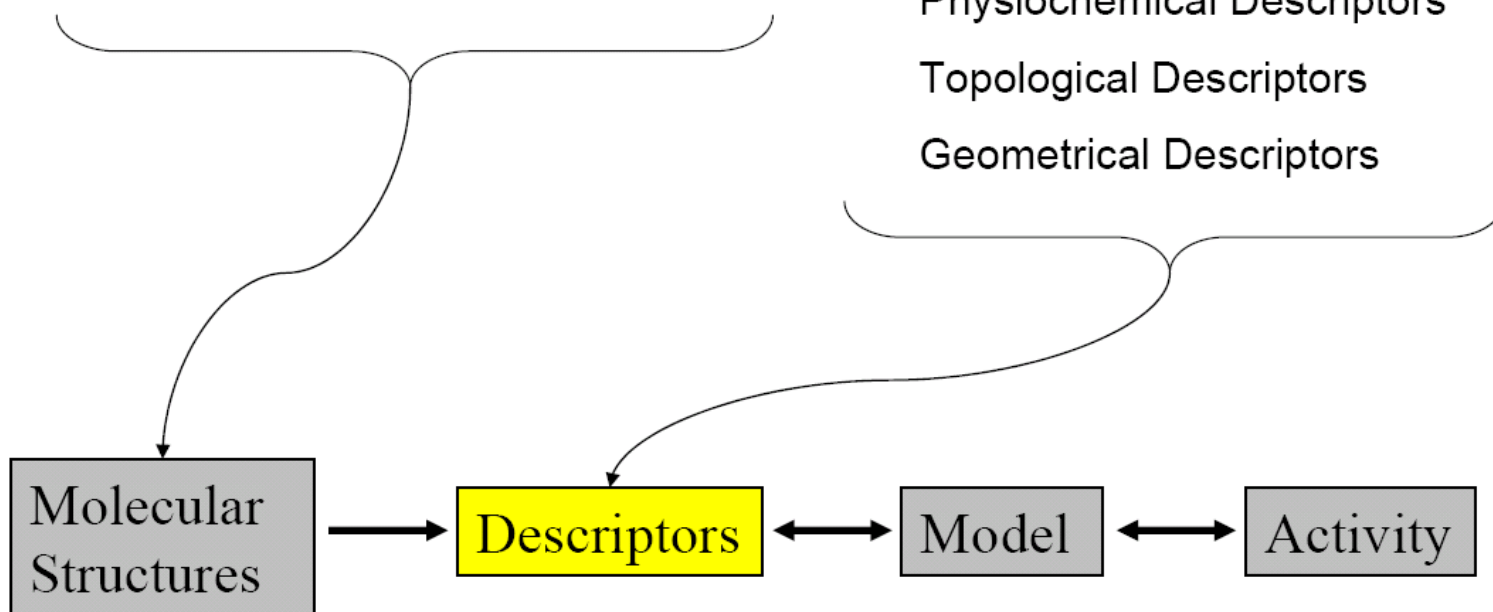
QSAR: What is AChE inhibition?
IC₅₀ is a measure of the concentration required for 50% inhibition.



Courtesy: Matt Sundling, RECCR Troy NY.



Structural Descriptors
Physiochemical Descriptors
Topological Descriptors
Geometrical Descriptors



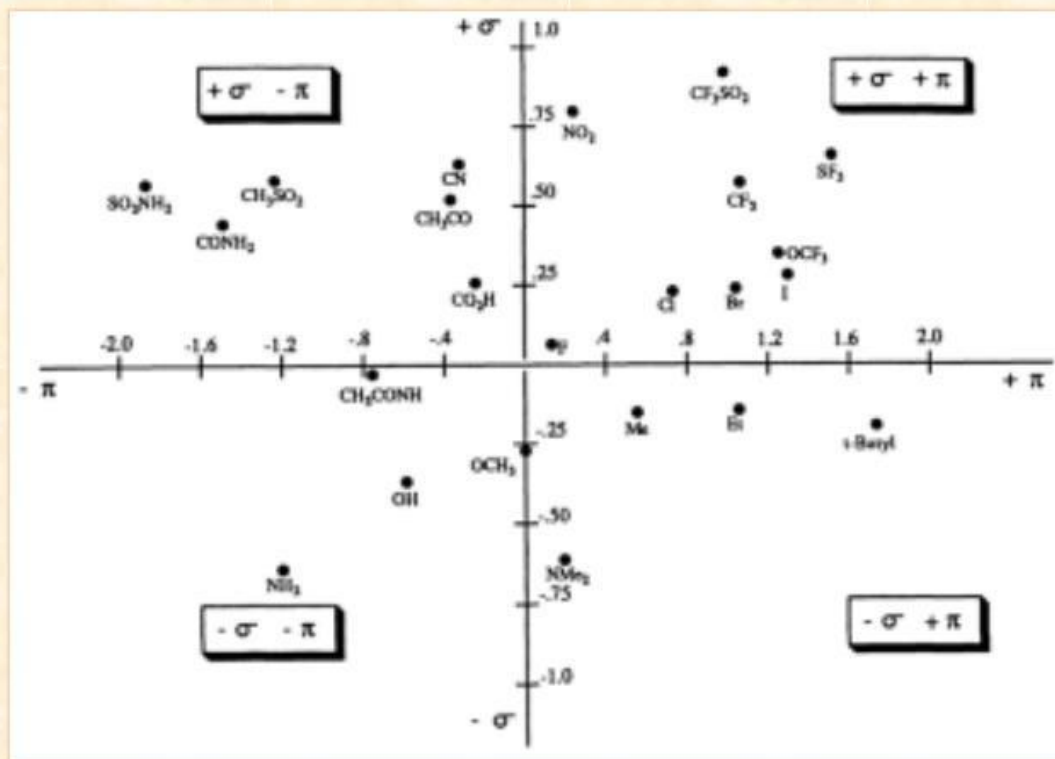
Courtesy: Matt Sundling, RECCR Troy NY.

Craig plot

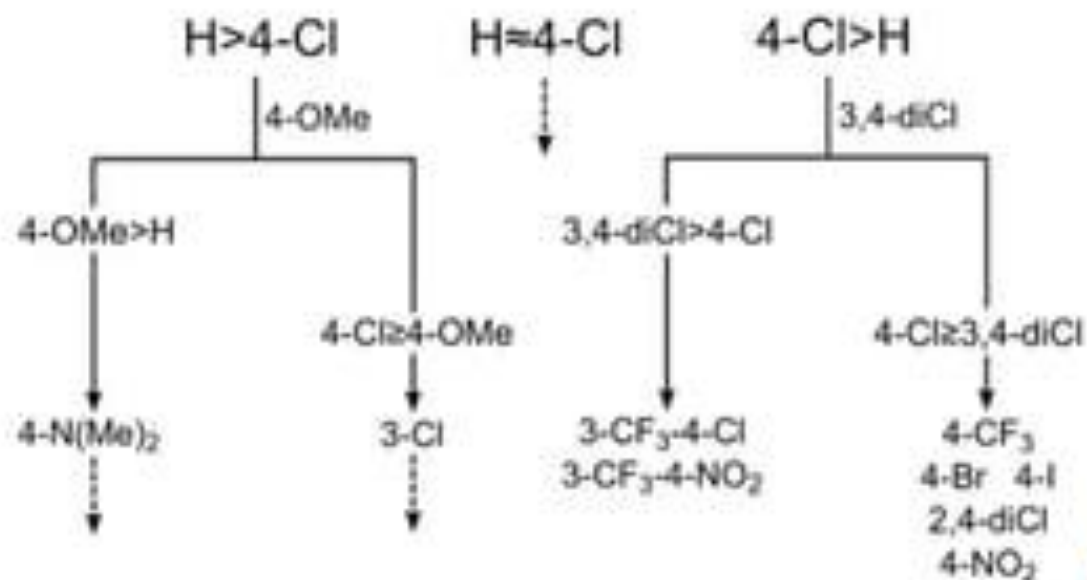
Tables of π & σ factors for different substituents are available.

However, easier to visualize **relative properties by considering a plot** with y-axis for σ & x-axis for π which is called **Craig plot**.

For example, Craig plot for para-aromatic substituents

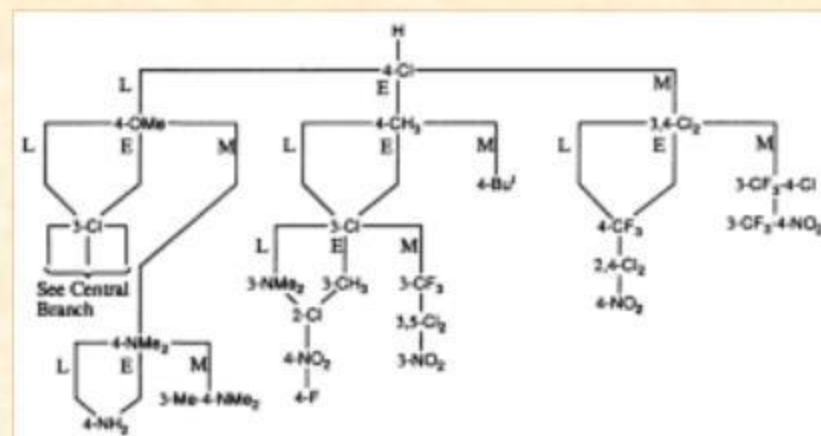


TOPLISS TREE FOR SUBSTITUTED PHENYL



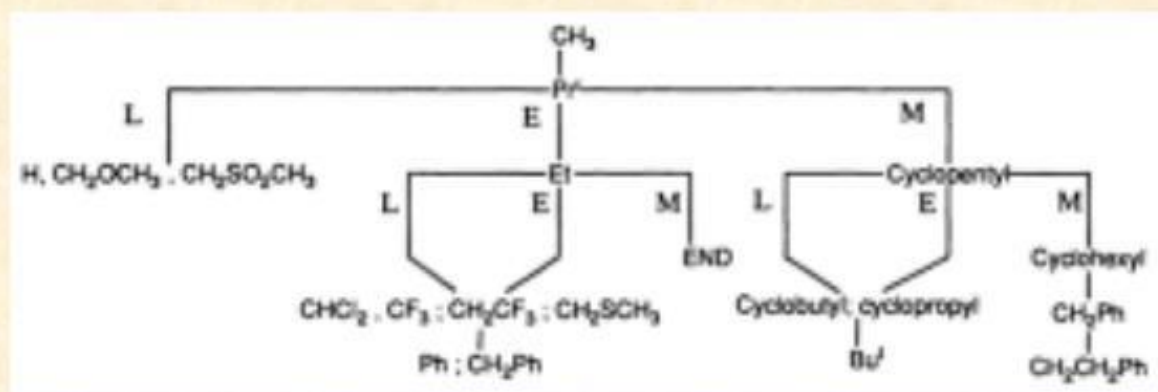
Topliss, J. G. Utilization of Operational Schemes for Analog Synthesis in Drug Design. *J. Med. Chem.* **1972**, *15*, 1006-1011.

Topliss scheme



Topliss scheme for aromatic substituents

Topliss scheme



Topliss scheme for aliphatic side chain substituents