doi: http://dx.doi.org/10.4172/2155-9554.S1.01

OMICS Group Conferences
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International Conference & Exhibition on
Clinical Research
Dermatology, Ophthalmology & Cardiology
5-6 July 2011 San Francisco, USA

Fractal dimension of transdermal-delivery drug models: 4-alkylanilines

Francisco Torrens
Universidad Católica de Valencia, Spain

The pathways that exist in porous membranes used to deliver drugs form *fractal* percolating paths. For a homologous series of 4- alkylanilines, the *fractal dimension D* is calculated as a model for transdermaldelivery drugs. Program TOPO is used for the calculation of the *solvent-accessible surface* AS, which is denoted by the centre of a probe, which is allowed to roll on the outside while maintaining contact with the *bare* molecular surface *S*. AS depends on the probe radius *R*. For 4-alkylanilines, the quadrupole moment ı is doubled. The hydrophobic contribution to AS is doubled while its hydrophilic part remains constant. *D* increases 11%. Geometric descriptor and topological index results are in agreement with reference calculations. The 1-octanol– water partition coefficient log*P* increases. The molar concentration of organic compounds necessary to produce a 1:1 complex with bovine serum albumin *via* equilibrium dialysis, log1/*C* increases. The hydrophile–lipophile balance (HLB) decreases. The linear correlation between *D* and ı, and non-linear correlations between *D*, log*P*, log1/*C* and HLB point to a homogeneous molecular structure of the 4-alkylanilines. The comparison with phenyl alcohols shows that their greater dipole moments cause lower hydrophobicity.