International Conference & Exihibition on
Analytical and Bioanalytical Techniques 2010
ANANBIOANAL - 2010
Pharmaceutical R & D Summit
doi:10.4172/2155-9872.1000060

QSAR and Drug Designing for Anti-Tumor/Anti-Cancer Activity

Rama Pande

School of Studies in Chemistry, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh, India

QSAR is the science which relates chemical structure of biological activity. N-arylphydroxamic acids of general formula, $R_1NOH.R_2C=0$, where R_1 and R_2 are phenyl or/and substituted phenyl groups are biomolecules as (i) They follow the "Lipinski Rule of 5", (ii) Contain both HBD and HBA sites. These molecules are neutral polyfuncitonal molecules and hydrogen-bonds helps in drug delivery system by providing binding interaction with receptors. The hydrophobic, electronic and steric parameters of 20 such molecules are derived following the experimental techniques along with computation methods. The antiproliferative effect of these molecules was studies in-vitro and and in-vivo. The biological parameters like concentration, time intervals and survival period are also measured. Based on these data the mechanism of death of cancerous cell is studied under the heads, (i) ROS, (ii) Mitochondrial potential (iii) Lipid peroxidation and (iv)DNA Ladder. The QSAR parameters determined are correlated with biological activity estimated, following the MRA and PLS methods and the potency of molecules are computed, by formulating and generating the equations for the molecules under study. All the molecules investigated show anti-tumor activity when tested in-vitro. One molecule, N-p-Chlorophenys-4-bromobenzohydroxamic acid with best IC_{50} value (53 micro molar) is selected for in-vivo experiments. The results show that 100 mg of this molecule kills 90% cancerous cells in 16 days, per kg. wt. of mice with the clean death of cancerous cells.