MM005-DIBENZOYLMETHANES: HANSCH ANALYSIS FOR THE INIBITION OF MCF7 CELL LINES.

QUIRINO A. DE LIMA NETO(IC)[1]; RALPHO R. DOS REIS(PQ)[1]; MARISA A. NOGUEIRA(PQ)[1]; EDUARDO B. DE MELO(PQ)[1].

[1] – UNIOESTE - Curso de Farmácia - Universidade Estadual do Oeste do Paraná (UNIOESTE)[1]

The breast cancer constitute the first cause of women's death in Brazil. The dibenzoylmethanes are a rare group of flavonoyds which presents anticancer activities *in vitro*. This trial on carrying out a Hansch Analysis of a set of nine compounds sintetized and ensaied for Nogueira *et al* for the inibition of MCF7 breast cancer cell lines. The structures were optimized at AM1 level in the Hyperchem. Fourty five descriptors (30 electronics, 12 sterics and 3 hydrophobics) were evaluate. The Log %TI (percentage of total inhibition) was the dependent variable. The QSAR was performed in the BuildQSAR. The best models with a single descriptor were: (I) -0.1850 LogP + 2.8803 (r=0.912; s=0.083; q^2=0.701) e (II) -0.0119 MR +3.1360 (r=0.858; s=0.103; q^2=0.565). Values of *r* and q^2 were best for (I), however, the *r* for external validation with a set of three compounds (-0.70 and -0.67, respectively) showed that the equations presents practically the same capacity of prediction. These models demonstrate that hydrophobics and sterics factors are important for the described activity, with bigger prominence for the first one, what already it was observed in anothers works.

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MM006- CONSTRUCTING PROTEIN PRUNING MODELS TO PERFORM RECEPTOR-DEPENDENT (*RD*) 4D-QSAR ANALYSIS OF A SET OF DIAZABORINE DERIVATIVES

KERLY FERNANDA MESQUITA PASQUALOTO[1] (PQ); MÁRCIA MIGUEL CASTRO FERREIRA[1] (PQ); OSVALDO ANDRADE SANTOS-FILHO[2] (PQ) ; ANTON J. HOPFINGER[2] (PQ)

[1] UNICAMP
[2] UIC

Introduction: Receptor pruning is an approach for achieving reasonable conformational ensemble profile and performing practical *RD* 4D-QSAR analysis in terms of time and computational resources. Purpose: Reduce the size of a model structure of enoyl-acp reductase (ENR) from *E. coli*, FabI, to allow ligand-receptor molecular dynamic simulations (MDSs) to be computationally economical yet still provide meaningful binding thermodynamic data. Methodology: Three reduced-size models of FabI were created by pruning away all residues greater than 12, 10 and 8 Å radius. The largest ligand was docked in the active site to define the largest required receptor model. Energy minimization and MDSs were carried out using the MOLSIM 3.2 program. The lowest energy structure for each of receptor models from MDSs was compared by root mean square (RMS) fit to the equivalent portion of the crystal structure of FabI. Results: A scale-down 12 Å receptor model of the enzyme FabI maintains the structural integrity of the composite parent crystal structure. Perspectives: Structure-based design of new antituberculosis agents regarding the similarity in the active site of two ENRs, FabI and InhA (*M. tuberculosis*).

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