

MM - Modelagem Molecular

Molecular Modeling

MM001	VALIDATION OF SEMI-EMPIRICAL METHODOLOGY FOR GEOMETRY OPTIMIZATION OF HIV-IN INHIBITORS	EDUARDO B. DE MELO (PG) ¹ ; ALINE T. BRUNI(PQ) ² ; MÁRCIA M. C. FERREIRA(PQ) ³	EDUARDO BORGES DE MELO
MM002	TRYPANOTHIONE-REDUCTASE: DOCKING STUDIES OF PEPTIDE ANALOG INHIBITORS	SAMUEL SILVA DA ROCHA PITA (PG) ¹ ; MAGALY GIRÃO ALBUQUERQUE (PQ) ¹ ; JOSÉ JAIR VIANNA CIRINO (PQ) ¹ ; RICARDO BICCA DE ALENCASTRO (PQ) ¹ ; CARLOS RANGEL RODRIGUES (PQ) ¹ ; HELENA CARLA CASTRO (PQ) ¹	SAMUEL SILVA DA ROCHA PITA
MM003	AM1 SEMI-EMPIRICAL STUDY IN THE OPTIMIZATION OF PRODRUGS WITH POTENTIAL ANTICHAGASIC ACTIVITY	GUSTAVO H. G. TROSSINI (PG); ELIZABETH I. FERREIRA (PQ); CARLA M. S. MENEZES (PQ)	GUSTAVO H. G. TROSSINI
MM004	QSAR STUDY OF PIPERINE AND THEIR ANALOGUES WITH THE AID OF CHEMOMETRIC TOOLS	HELLEN M. OLIVEIRA (IC); PRISCYLA R. MENDANHA (IC); GILBERTO L. B. AQUINO (PQ); MARCELO M. SENA (PQ).	PRISCYLA R. MENDANHA
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 .	QUIRINO A. DE LIMA NETO
MM006	CONSTRUCTING PROTEIN PRUNING MODELS TO PERFORM RECEPTOR-DEPENDENT (RD) 4D-QSAR ANALYSIS OF A SET OF DIAZBORINE DERIVATIVES	KERLY FERNANDA MESQUITA PASQUALOTO ¹ (PQ); MÁRCIA MIGUEL CASTRO FERREIRA ¹ (PQ); OSVALDO ANDRADE SANTOS-FILHO ² (PQ) ; ANTON J. HOPFINGER ² (PQ)	KERLY FERNANDA MESQUITA PASQUALOTO
MM007	A HCA STUDY FOR ANTIMUTAGENIC ACTIVITY OF DIBENZOYLMETHANES IN SALMONELLA TYPHYMURIUM.	MARCELO C. FRIOZI(IC); QUIRINO A. DA LIMA NETO(IC); RALPHO R. DOS REIS(PQ); MARISA A. NOGUEIRA(PQ); EDUARDO B. DE MELO(PQ).	MARCELO COUTO FRIOZI
MM008	AZASUGARS: A CORRELATION STUDY BETWEEN α -GLUCOSIDASE INHIBITION VS ELECTRONIC DESCRIPTORS	RICARDO LORENZONI (IC); EDUARDO B. DE MELO (PQ).	RICARDO LORENZONI
MM009	APPLICATION OF UNSUPERVISED CHEMOMETRICS METHODS TO A SET OF INHIBITORS OF ESCHERICHIA COLI ENOYL-ACP REDUCTASE, FABI	FLÁVIA DA SILVA PEREIRA ¹ (PG); WALKÍRIA RÉGIS DE MEDEIROS ¹ (PG); KERLY FERNANDA MESQUITA PASQUALOTO ¹ (PQ); MÁRCIA MIGUEL CASTRO FERREIRA ¹ (PQ)	FLÁVIA DA SILVA PEREIRA