Nuttapong Ithiapa 2012: Comparative Molecular Field Analysis and Quantum Calculation Study on Anti HIV-1 RT Diarylaniline Derivatives. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Mr. Songwut Suramitr, Ph.D. 78 pages.

The goal of the research is the demonstrating the cause of the diarylaniline derivative drugs resistance using the CoMFA and quantum chemical calculations. Over all obtained results can be used to guide the new designed potent anti HIV-1 Reverse Transcriptase inhibitors for enzyme. In this study, the relationship between structural properties of 25 diarylaniline derivatives and their 50% effective concentrations (EC_{50}) to HIV-1 Reverse Transcriptase (RT) using a comparative molecular field analysis (CoMFA) were constructed. The best predictive CoMFA model gives a very good statistical result with r_{cv}^2 = 0.823, r_{nv}^2 = 0.924, S_{press} = 0.422, *SE* = 0.241, *F* = 65.055, steric contribution = 28.1% and electrostatic contribution = 71.9%. Consequently, the obtained CoMFA contour maps merging with the wild type HIV-1 RT binding site can give the informative details for understanding the structural requirements of inhibitors and can guide the new design of diarylanilline inhibitors. Deeply in molecular details, an understanding of particular interaction energy between antiHIV-1 inhibitors and surrounding residues in the binding pocket was performed by using B3LYP, M062X and MP2/6-31G(d,p) calculations. These calculations technical demonstrated the rationality of our hypothesis about main interaction between diarylaniline derivative and HIV-1 Reverse Transcriptase. The obtained results clearly demonstrate that compound 24 have more interaction and more efficiency than compound 1.

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