International Journal of Innovative
Computing, Information and Control
Volume **5**, Number **7**, July **2009**

ICIC International ©2009 ISSN 1349-4198
pp. **2061–2070**

DRUG DESIGN VIA NOVEL DIRECTIVITY GENETIC ALGORITHMS AND LYAPUNOV PRINCIPLE

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Received January 2008; revised June 2008

Abstract. *This investigation presents novel computer graphical and computational schemes for solving the challenges of a computer-aided drug design (CADD). The application of the energy minimum to enhance the docking performance of CADD is discussed in terms of three aspects, geometry, energy and activity. This study applies the energy minimum theorem to solve the objection. A geometry search is performed and compared with four types in classification of receptors. First, this work attempts to improve the speed of computer simulations of protein folding, and proposes an improved genetic algorithm to accelerate the binding site search; next, we focus on energy theme. Lyapunov's stability theorem is adopted to decrease the number of binding sites, thus enhancing the docking performance in computer simulation examples. Finally, various drug-ligand interaction models are employed to compute docking simulation, and energy minimum theorem is used to judge the approach global energy minimum area and docking stability. The significance of the eigenvalue λ is analyzed at each protein folding, and the performance has increased by 25 percents compared with various binding sites. Additionally, the protein folding and various bond forces in drug-ligand interaction model are discussed. Comparing four optimal geometry search methods and referring to Pegg and Camila's previously published papers in benchmark of drug docking database, the improved genetic algorithms are specified to undertake the search binding site and docking, and the global minimum search and the arithmetic convergence time of 1.16hr are achieved. Analytical results indicate that the improved genetic algorithm is better than that of traditional random methods in terms of processing the geometry graphics operation.*

Keywords: Lyapunov equation, Minimum energy, Improved genetic algorithms

1. **Introduction.** The National Institute of Allergy and Infectious Diseases (NIAID) of the American National Institutes of Health (NIH) has found an increase in disease, resulting in a need to accelerate drug discovery, although commercializing a new drug is extremely complicated [2]. In addition to these natural infections, the accidental or intentional spread of microbes, as in the 2001 anthrax attack, 2003 SARS, 2005 Avian Influenza, further complicates the difficult challenge of protecting public health. The average drug development time is 14.9 years, and the average development cost is US-$802 million dollars to progress from the research laboratory to use by patients, according to a 2004 report from the J. Health Econ and the Tufts Center for the Study of Drug Development [3]. In response to the above challenges that shorten drug development time and employing rapid advances computer technologies to cut down cost is very important key point. [4] Computer-aided drug design (CADD) will be a crucial and significant