MODELING AND DOCKING STUDIES OF BIOLOGICAL DATA STAT4 INVOLVED IN CANCER

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ABSTRACT

The amount and variety of data in natural sciences increases rapidly. Data abstraction, Data manipulation and Pattern discovery techniques are of great need in order to deal with such large quantities. Integration between different sources of data is also of major interest, as complex relations may arise. Biology is a good example of a field that provides extensive, highly variable and multi-sources data. The technical advances achieved by the genomics, metabolomics, transcriptomics and proteomics technologies in recent years have significantly increased the amount of data that are available for biologists to analyze different aspects of an organism. Bioinformatics is an interdisciplinary research area at the interface between computer science and biological science.

In order to identify a better drug for cancer, STAT4 (signal transducers and activators of transcription) protein was choosed as target. A three dimensional (3D) model of the STAT4 is generated based on the crystal structure of 1Y1U template by using Modeller software. With the aid of the molecular mechanics and molecular dynamics methods, the final model is obtained and is further assessed by Procheck and Verify 3D graph programs, which showed that the final refined model is reliable. With this model, a flexible docking study is performed with different drugs. From the docking studies, we also suggest that MET3, ARG4, THR5 in STAT4 domain are three important residues in binding. The hydrogen bonding interactions play an important role for stability of the complex. Our results may be helpful for further experimental investigations.

KEYWORDS: Biological Data, Cancer, Docking Studies, Naphazoline, Modeling and STAT4