Universitas Indonesia Library >> Artikel Jurnal

In Silico Approach to Finding New Active Compounds from Histone Deacetylase (HDAC) Family

Arry Yanuar, author

Deskripsi Lengkap: http://lib.ui.ac.id/detail?id=20461474&lokasi=lokal

---

Abstrak

ABSTRACT
Histone Deacetylase (HDAC) enzymes in the human body play an important role in the transcriptional regulation of gene expression. In the last decade, HDAC inhibitors and activators have been explored and have become known as therapeutic agents for many diseases such as osteodystrophy, neurogenerative disorders, cardiomyopathy, cancer, and diabetes. In recent years, the development of HDAC inhibitors or activators to obtain new potent lead compounds has been conducted using in vitro, in vivo, and in silico methods. Some HDAC family inhibitors and activators have been discovered. But some compounds have limitations such as not selectively binding to one of the HDAC variants. Methods: At present, through bioinformation, HDAC family sequences have been revealed, and some in silico methods such as molecular modelling (homology modelling and pharmacophore modelling), virtual screening, and molecular dynamics are widely used to find and develop new potent and selective compounds. Results: The main utilization of molecular modelling in this work is intended to complete the HDAC structure that partially lacks data regarding its amino acid monomer. Virtual screening methods are helpful in finding the best binding affinity of the test compounds. By molecular dynamic simulation, the temperature, time, and pressure can be adjusted to analyze the hydrogen bond. Conclusion: Combining these in silico approaches will be a more effective and efficient solution in finding new lead compounds for HDAC drug discovery research in the future