OMICS Group Conferences
Accelerating Scientific Discovery

2nd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing

October 15-17, 2013 Hampton Inn Tropicana, Las Vegas, NV, USA

Novel drug design for Alzheimer's disease by in silico approach

Jyothi Vanama[1], G. Girija Sankar[1], C.Sundaramoorthi[2] and A. Raja Sekaran[2]
[1]Andhra University, India
[2]KMCH College of Pharmacy, India

Alzheimer's disease (AD) is a common neurodegenerative disorder associated with dementia in late adulthood. Apolipoprotien E, a multifunctional protein with central roles in lipid metabolism and neurobiology, has three common isoforms (apoE2, apoE3, apoE4) with different effects on lipid homeostasis and neurobiology. Unlike apoE3 which is the most common isoform, apoE4, is associated with increased risk of developing AD and other neurodegenerative disorders. Even though the molecular level of mechanisms underlying the apoE's role is not clear, it is evident from the various research data that the apoE's interact with various factors in different pathways. Thus, an alternative to traditional drug discovery was chosen for designing anti-AD drugs by understanding the structure of the apoE and its impact on the neurodegenerative process by in silico approach to genome analysis and similar protein structure was predicted. Our novel molecular level bioinformatics screening system comprised of various independent assessment procedures that included

1. Determining the structure of apoE gene
2. Building a Swiss PDB model of binding site
3. Search databases for modeled site
4. Dock new guests and binding sites
5. Predicting binding constants
6. Constructing the Ligand

We have discovered ten similar molecules for drug-targetable apoE structure by applying selective in silico approach.

Results: The results obtained showed that 2-Phenyl-4-quinolinamine is interacting at the lowest energy level with all the amino acids in the potential active site. Findings from this work suggest that 2-phenyl 4-quinolinamine could be the lead molecule in the treatment for AD.

jpk1305@gmail.com