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Structural designing of suppressors for autisms spectrum diseases using molecular dynamics sketch

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Abstract

In this paper we are sketching the chemical structure of suppressor drug for autism spectrum disorder using a computational tool .Here we are designing three molecular compounds like Fluoxetine, Risperidone, Melatonin .Structuring the suppressors, sketching the aromatization and bonding of the functional groups withthe elements like Oxygen ,Nitrogen ,halogens. In our work we are using computational algorithm for drawing the structure of suppressor drug. In this paper we are mentioning the autism spectrum suppressor's molecular formula as well as structural formula.

Keywords: Cheminformatics, Drug designing, Autism, Fluoxetine, Risperidone, Melatonin.

Introduction

Cheminformatics is a technique which incorporate the Computer Science, Machine learning and chemistry mainly used for the drug prediction and drug discovery. It is branch of science which deal to solve the chemical drug related pattern using the modern approach. It also focuses on storing, extracting and indexing the chemical components. A Cheminformatics methodology has been adopted mainly in pharmaceutical for drug designing and discovery. [1] It has now emerged as an inevitable part in modern drug discovery. It uses computational method for designing and predicting the drug structure.

Cheminformatics is a science that deals discovering and developing the drugs using [2] modern drug developing technologies that helps us to clear the faults or bugs that are present in the traditional drug development technologies. Designing a drug to is very complex task. [3] There are very few drugs which have efficient but have very less accuracy. But the accuracy of such drugs can be improved using the [4] Cheminformatics technology and thereby increasing the efficiency of the drug.

Review of literature

Cheminformatics deals with discovering drugs based in modern drug discovery methods which in turn rectifies complex issues in traditional drug discovery system.[5] Cheminformatics tools supports medical chemist for better understanding of complex structures of chemical compounds. : Jie Dong [6] projected that numerous tools have been developed to represent these components.

However, they have some restrictionsie they only concentrate on the analysis of either small molecules or proteins or DNAs/RNAs. Thus there is still absence of freely available, easy to use and unified platforms for generating molecular descriptors of DNAs/RNAs, proteins, small molecules and their interactions. A method to understand protein–chemical interactions using heterogeneous input consisting of both protein sequence and chemical information was proposed by: Misagh Naderi [7] in a graph-based approach to construct Target focused libraries for virtual screening. In the paper of Deep Belief Networks for Ligand-Based Virtual Screening of Drug Design by Aries Fitriawan [8] suggest about the virtual screening method in drug discovery the author talks about finding a new method for ligand-based virtual screening using machine learning technique here the classification has been done by using Deep Belief Networks (DBN) method which permit any inter-layer model of Restricted Boltzmann Machine (RBM) to receive a different depiction of the data from its output. Whereas the RBM is a simplification of the Boltzmann Machine models that have the energy formula of joint configuration. In Cheminformatics one of the important step in drug discovery is target prediction. : Zhonghua Wang [9] proposed that Silico target prediction of compounds plays insignificant role in drug discovery. After target Identification, validation phase starts by determining whether the modulation of the target will produce a desired clinical result.[10] Binary classifiers using the machine learning were developed for calculating the reactivity of potential substrates and products in the 12 classes of oxidoreductase-catalyzed reactions. [11] A technique to infer protein–chemical interactionsusing heterogeneous input consisting of both protein sequenceand chemical information.[12] user-friendly web-based software, named Drug-SN Ping, which provides a platform for the integration of drug information.[13] Several variant genotypes along with the development of Quasi-species restricted the effectiveness of drugs used for the treatment of HCV infections. This heterogeneity of the virus hindered the drug development against them. [14] The Latest

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study uses Ferric binding protein, which is used as a reference molecule to understand high reactive responses of various drugs administered for the oral periodontitis. The drugs are being compared with the Fbp. The Fbp interacted with doxycycline, flurbiprofen and chlorhexidine using docking methods. [10] Various computational methodologies have been suggested for the calculation of compound toxicity ranging from quantitative structure activity relationship modelling to molecular similarity-based approaches and machine learning.

Problem formulation

For autism spectrum disorder doesn't have specific proper drug to cure the diseases. [15] Tradition drug suppressor discovery methodadopted for the autism uses experimental methods and manual procedures which were time consuming and highly expensive. [16] The autism drug discovered using tradition methods was not efficient and accurate. Thus experiments has to be carried out several time in order to achieve the proper result.
[17]Using the Cheminformatics techniques it is possible to change the chemical structure of aautism drug with the perfect accuracy and efficiency by using the molecular dynamics concepts.

Problem definition

Autism is a spectrum of disorder which varies from one person to another person. Autism is a genetically disorder that are usually visible in children. There are very few drugs which could reduce the symptom. However these drug lack the accuracy and efficiency.
Our works aims to give awareness to public about the structure of autism spectrum disorder suppressors using molecular dynamics, sketching the suppressor and in future work we can redesign the suppressor to change the element positions and increase the efficiency.

COMPOUND NAME	MOLECULAR FORMULA
FLUOXETINE	$C_{17}H_{18}F_3NO$
MELATONIN	$C_{13}H_{16}N_2O_2$
RISPERIDONE	$C_{23}H_{27}FN_4O_2$

Table 1: Table For Drug Compound name and Molecular formula

The table 1 which given above is to describe the suppressors which we have taken for this paper work to sketch the structure

Flow diagram for drug designing of Asd

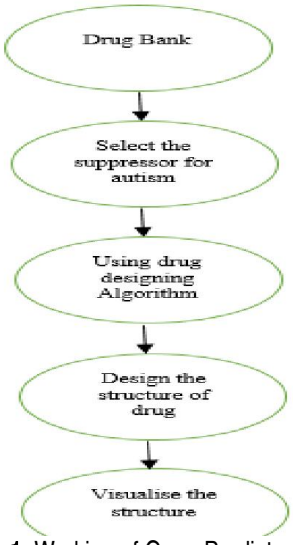

Figure 1: Working of Gene Predictor

Methodology

Input: mol file for the suppressor
1. Identify the suppressor.
2. Identify the focusing area of the drug on the autism.
3. Identify the aromatization and bonding the functional groups with the elements like Oxygen, Nitrogen, halogens.
4. dlg. Filter = *.moll*.moll*.cdxl*.cdxl*.cdxmll*.cdxmll*.rxnl*.rxnl*.mrvl*.mrvl*.cmll*.cmll*.mol2l*.mol2l*.tgfl*.tgfl*.smi";
5. if (dlg. Show Dialog())
6. using (Open File Dialogdlg = new Open File Dialog())
7. dlg. Filter = "*.sdfl*.sdf";
8. if (dlg. Show Dialog() == System. Windows. Forms. Dialog Result. OK)
9. sdf File. Text = dlg. File Name;
10..if (pe. Result!= System. Windows. Forms. Dialog Result. OK)
11.return;
12.structure = pe.Html;
13. Molecule m = Molecule. Read (structure);
14.string smiles = m. To String("smiles");
15.stringmolfile = m. To String ("molfile");
16.pictureBox1.Image = m. ToImage (pictureBox1.ClientSize.Width, pictureBox1.ClientSize.Height, 10);

The above psuedocode explains how to draw a chemical structure of the autism drug. The data relating to the existing drug has to be collected from ChEMBL in order to draw the structure. The extension has to be saved in mol or cdx, cd, cdxml etc. The drug has being designed in the picture box bydrag and drop method. The basic chemical structure has been mapped to the picture box.

Experimental result

DATASET:
These are the following suppressor which we are using for the experiment result

Compound ID	CHEMBL85
Compound Name	RISPERIDONE
ChEMBL Synonyms	Risperdal Consta Long Acting | R 64 766 | Risperdal consta | R-64766 | Risperdal M-TAB | R-64-766 | Risperdal | Risperdal M | RISPERIDONE
Trade Names	RISPERIDONE | Risperdal consta | Risperdal | Risperdal Consta Long Acting | Risperdal M-TAB | Risperdal M
Molecular Formula	$C_{23}H_{27}FN_4O_2$

Compound ID	CHEMBL41
Compound Name	FLUOXETINE
ChEMBL Synonyms	PROZAC WEEKLY | FLUOXETINE HYDROCHLORIDE | LY-110140 | SARAFEM | PROZAC | Sarafem | Symbyax | FLUOXETINE | Prozac
Trade Names	SARAFEM | FLUOXETINE HYDROCHLORIDE | PROZAC WEEKLY | FLUOXETINE | PROZAC
Molecular Formula	$C_{17}H_{18}F_3NO$

Compound ID	CHEMBL45
Compound Name	MELATONIN
ChEMBL Synonyms	N-ACETYL-5-METHOXYTRYPTAMINE | N-(2-(5-METHOXY-1H-INDOL-3-YL)ETHYL)ACETAMIDE | MELATONIN
Trade Names	unknown
Molecular Formula	$C_{13}H_{16}N_2O_2$

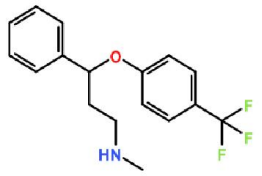

Figure 2:-The chemical structure of the Fluoxetine Drug

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The figure shows the chemical structure of the autism drug called fluoxetine. Fluoxetine is a drug which is under the clinical trial testing the efficiency of the drug. This aim of the drug to reverse avoidance behaviors and ameliorate social deficits. This drug is used to reduce the symptoms of the panic disorders.in this drug we are sketched aromatizationusing functional group halogens.

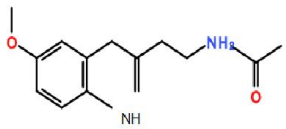

Figure 3:-The chemical structure of the Melatonin Drug.

The above structure represent the chemical structure of the 2nd suppressor drug called Melatonin. The drug targets the brain neurons causing the depression and sleeping disorder. This drug has been used for the treatment of the autism patient having the sleeping disorder and regulates the creation of hormones such as cortisol and serotonin. In this drug we are used aromatization using a functional group amine.

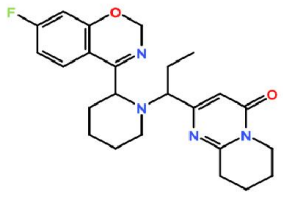

Figure 4: -The chemical structure of the Risperidone Drug.

The above figure depicts the chemical structure of the Risperidone drug which is an antidepressant drug which focuses on treating the autism children with aggression and self-injury tendencies. Thus there are several side effects for the particular drugs such as weight gaining. In this structure we have sketched aromatization with the various elements like N,O,F.

Conclusion

In this paper we are designing the suppressor drug for autism spectrum diseases using computational tool. Using molecular dynamics concept sketching the structural formula for suppressor using Cheminformatics and molecular dynamics methods.
We can extend the work, for redesigning these suppressors to change the functional group positions and consider the isomers of the same compound in that way we can increase the efficiency a proper drug for autism diseases using all the possible structural change with all permutations and combinations and reducing the side effects .

Conflict of Interest

The authors declare no conflict of interest.

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