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TITLE OF INVENTION	DEEP LEARNING-BASED METHODOLOGY FOR DEVELOPING MOLECULAR DOCKING TO GENERATE BETTER DOCKING SCORES
FIELD OF INVENTION	CHEMICAL
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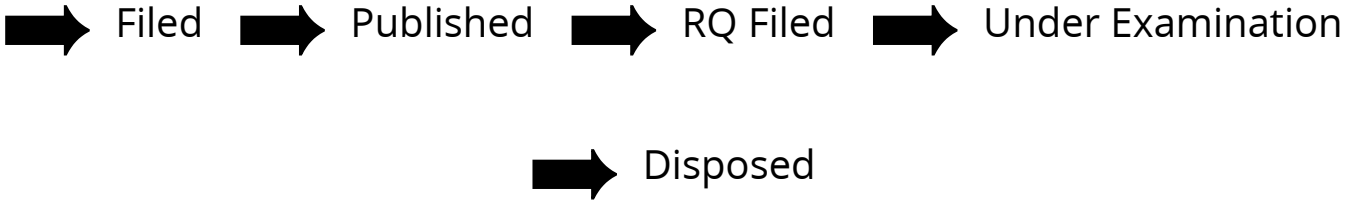

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FORM 2

THE PATENT ACT 1970

(39 OF 1970)

AND

The patent rules, 2003

COMPLETE SPECIFICATION

(See section 10: rule 13)

TITLE OF INVENTION

Deep learning-based methodology for developing molecular docking to generate better docking scores

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PREAMBLE TO THE DESCRIPTION

COMPLETE

Following specification particularly describes the invention and the manner in which it is to be performed.

Technical field of invention:

The present inventionrelates deep learning-based methodology for developing molecular docking to generate better docking scores.

Prior Art:

DK2381382T3 discloses a method for the prediction of adverse cross-reactions between lead candidate biomolecules and potential reactant molecules, often biopolymers, is described. In a computational system, reactions are modeled within a suitable environment, in order to determine a reaction profile between a lead candidate molecule and a potential reactant molecule. A risk assessment is then generated for each lead based on a plurality of reaction profiles for the lead with respect to a plurality of potential reactant molecules. The method includes provision for the redesign and optimization of the lead candidate, possibly iterative in nature, in order to avoid predicted adverse cross-reactions.

JP2017123169A aims to provide a method of predicting adverse cross-reactions between lead candidate biomolecules and potential reactant molecules, often biopolymers, in order to better characterize lead candidates in terms of safety and efficacy as pertains to a target disease or biological condition and to avoid adverse and/or otherwise unanticipated cross reactions with other unrelated biomolecules. In a computational system, reactions are modeled within a suitable environment in order to determine a reaction profile between a lead candidate molecule and a potential reactant molecule. A risk assessment is then generated for each lead based on a plurality of reaction profiles for the lead with respect to a plurality of potential reactant molecules. The lead candidate is iteratively redesigned and optimized in order to avoid predicted adverse cross-reactions.

US20160292394A1 discloses a method for partitioning a molecular subset is described. The partitioning method takes into account molecular structure and its manner of storage and transmission, transformations to be applied to the molecular subset and their implementation, and constraints imposed by the implementation of the partitioning method. Using this method, a molecular subset can be stored, transmitted, and processed more efficiently. The resulting efficiency makes it possible to design and run applications which require complex molecular processing, such as rational drug discovery, virtual library design, etc.

US11080570B2 discloses systems and methods for test object classification are provided in which the test object is docked with a target object in a plurality of different poses to form voxel maps. The maps are vectorized and fed into a convolutional neural network comprising an input layer, a plurality of individually weighted convolutional layers, and an output scorer. The convolutional layers include initial and final layers. Responsive to vectorized input, the input layer feeds values into the initial convolutional layer. Each respective convolutional layer, other than the final convolutional layer, feeds intermediate values as a function of the weights and input values of the respective layer into another of the convolutional layers. The final convolutional layer feeds values into one or more fully connected layers as a function of the final layer weights and input values. The one or more full connected layers feed values into the scorer which scores each input vector to thereby classify the test object.

US10874678B2 invention provides novel polydentate selective high affinity ligands (SHALs) that can be used in a variety of applications in a manner analogous to the use of antibodies. SHALs typically comprise a multiplicity of

ligands that each bind different region son the target molecule. The ligands are joined directly or through a linker thereby forming a polydentate moiety that typically binds the target molecule with high selectivity and avidity.

US9394303B2 invention is in the field of medicinal chemistry. In particular, the invention relates to a new class of small-molecules having pyrazolo pyridine structure which function as inhibitors of Mcl-1 protein, and their use as therapeutics for the treatment of cancer and other diseases.

CN103502458B Illustrate targeting and/or the method for cellular uptake efficiency of a kind of viral vector changing adeno-associated virus (AAV) at this, this viral vector has a kind of capsid comprising AAV9 cell surface binding structural domain. The method relates to modifying a clade F cell surface receptor, and this receptor comprises a kind of polysaccharide, and this polysaccharide has a terminal sialic acid residue and a β galactose residue second from the bottom. This modification can relate to making this carrier targeting again by the most functionally removal AAV9 combination in a cell subsets, thus this carrier is pointed to another cell subsets again. Alternately, this modification can relate to increasing cellular uptake efficiency to expose cell surface β galactose by processing these cells with a kind of neuraminidase. The numerous compositions containing AAV9 carrier and neuraminidase isadditionally provided at this. The method that the β galactose that a kind of use is connected on solid support carries out purification AAV9 is additionally provided at this. Additionally provide various mutations carrier at this, these mutational vectors have been modified to change their targeting specific, and they include: mutant AAV9, and wherein galactose binding structural domain is undergone mutation And AAV, one of them AAV9 galactose binding structural domain is engineered.

US20200277597A1 discloses methods for identifying bio-molecules with desired properties (or which are most suitable for a round of directed evolution) from complex bio-molecule libraries or sets of such libraries. Some embodiments of the present disclosure provide methods for virtually screening proteins for beneficial properties. Some embodiments of the present disclosure provide methods for virtually screening enzymes for desired activity and/or selectivity for catalytic reactions involving particular substrates. Some embodiments combine screening and directed evolution to design and develop proteins and enzymes having desired properties. Systems and computer program products implementing the methods are also provided.

KR101341876B1 invention relates to algorithms and methods for designing inhibitors that covalently bind a target polypeptide. The algorithms and methods can be used to quickly and efficiently convert reversible inhibitors into irreversible inhibitors.

US9676749B2 disclose compositions and methods for cancer detection and treatment. Compounds that inhibit PRMT5 are contemplated, as are pharmaceutical compositions comprising a therapeutically effective amount of at least one PRMT5 inhibitor. In some embodiments pharmaceutical compositions further comprising at least one HDAC inhibitor are contemplated. Methods of treating disorders in a mammal by inhibiting PRMT5 by administering to a mammal, a therapeutically effective amount of a PRMT5 inhibitor are also disclosed.

US10529003B2 discloses an optical bio module for detecting a disease specific biomarker(s), utilizing enhanced fluorescence emission (due to integration of a three-dimensional (3-D) protruded structure (s)) in a fluidic container/zero-mode waveguide, upon chemical binding of a disease specific biomarker(s) with

its corresponding disease specific biomarker binder(s) (e.g., an aptamer(s)) is disclosed.

JP2021042209A disclose methods for identifying compounds capable of binding to GPCRs in functional conformation states. Disclosed is a method comprising the steps of: a) providing a GPCR and a protein binding domain that can bind to a conformational epitope of the GPCR where the protein binding domain comprises a nanobody or an appropriate fragment thereof; b) forming a complex comprising the protein binding domain and the GPCR where the GPCR is in a functional conformational state; c) providing a test compound; d) evaluating whether the test compound binds to the GPCR in the functional conformational state or not; and e) selecting the compound that binds to the GPCR in the functional conformational state.Molecular Docking is a strategy to examine the conformation and orientation to binding site of a specific macromolecule. Recent years have seen a huge adoption of docking techniques both in academic and industrial arenas due to its accuracy and reduced cost.

Groupings of alternative elements or embodiments of the invention disclosed herein are not to be construed as limitations. Each group member can be referred to and claimed individually or in any combination with other members of the group or other elements found herein. One or more members of a group can be included in, or deleted from, a group for reasons of convenience and/or patentability. When any such inclusion or deletion occurs, the specification is herein deemed to contain the group as modified thus fulfilling the written description of all Markush groups used in the appended claims.

The recitation of ranges of values herein is merely intended to serve as a shorth and method of referring individually to each separate value falling within the range. Unless otherwise indicated herein, each individual value is incorporated

into the specification as if it were individually recited herein. All methods described herein can be performed in any suitable order unless otherwise indicated herein or otherwise clearly contradicted by context.

The use of any and all examples, or exemplary language (e.g. “such as”) provided with respect to certain embodiments herein is intended merely to better illuminate the invention and does not pose a limitation on the scope of the invention otherwise claimed. No language in the specification should be construed as indicating any non-claimed element essential to the practice of the invention.

The above information disclosed in this Background section is only for enhancement of understanding of the background of the invention and therefore it may contain information that does not form the prior art that is already known in this country to a person of ordinary skill in the art.

Objective of the invention

The primary object of thepresent invention isdeep learning-based methodology for developing molecular docking to generate better docking scores.

Summary of the invention:

Accordingly following invention is deep learning-based methodology for developing molecular docking to generate better docking scores.

Brief description of drawings

Further clarify various aspects of some example embodiments of the present invention, a more particular description of the invention will be rendered by reference to specific embodiments thereof which are illustrated in the appended drawings. It is appreciated that these drawings depict only illustrated embodiments of the invention and are therefore not to be considered limiting of its scope. The invention will be described and explained with additional specificity and detail through the use of the accompanying drawings.

In order that the advantages of the present invention will be easily understood, a detail description of the invention is discussed below in conjunction with the appended drawings, which, however, should not be considered to limit the scope of the invention to the accompanying drawings, in which:

Figure 1 shows a block diagram representation ofdeep learning-based methodology for developing molecular docking to generate better docking scoresaccording to the present invention.

Detailed description of invention:

The following description includes the preferred best mode of one embodiment of the present invention. It will be clear from this description of the invention that the invention is not limited to these illustrated embodiments but that the invention also includes a variety of modifications and embodiments thereto. Therefore, the present description should be seen as illustrative and not limiting. While the invention is susceptible to various modifications and alternative constructions, it should be understood, that there is no intention to limit the invention to the specific form disclosed, but, on the contrary, the invention is to cover all modifications, alternative constructions, and equivalents falling within the spirit and scope of the invention as defined in the claims.

In any embodiment described herein, the open-ended terms "comprising," "comprises," and the like (which are synonymous with "including," "having" and "characterized by") may be replaced by the respective partially closed phrases "consisting essentially of," consists essentially of," and the like or the respective closed phrases "consisting of," "consists of, the like.

The present invention relates deep learning-based methodology for developing molecular docking to generate better docking scores.

Method:

1. Initially a small set of molecules are docked from which the validation set, training set and test data sets of molecular samples are extracted.

2. These data sets are used for predicting the docking patterns in the large database in Bigdata.

3. The database is reduced and subject to random sampling.

4. An improved docking model is generated by training the small sample of molecules.

5. Based on the improved model, effective prediction is done on Bigdata using Quantitative Structure Activity Relationship Descriptors.

6. After database reduction, the virtual hit counts are updated and are subject to random sampling until high docking scores are generated.

Additional advantages and modification will readily occur to those skilled in art. Therefore, the invention in its broader aspect is not limited to specific details and representative embodiments shown and described herein. Accordingly various modifications may be made without departing from the spirit or scope of the general invention concept as defined by the appended claims and their equivalents.

We Claims:

1. The present invention relatesdeep learning-based methodology for developing molecular docking to generate better docking scores.

2. Deep learning-based methodology for developing molecular docking to generate better docking scores claimed in claim 1,various steps of method:

    i. Initially a small set of molecules are docked from which the validation set, training set and test data sets of molecular samples are extracted.

    ii. These data sets are used for predicting the docking patterns in the large database in Bigdata.

    iii. The database is reduced and subject to random sampling.

    iv. An improved docking model is generated by training the small sample of molecules.

    v. Based on the improved model, effective prediction is done on Bigdata using Quantitative Structure Activity Relationship Descriptors.

    vi. After database reduction, the virtual hit counts are updated and are subject to random sampling until high docking scores are generated.

Abstract

The present invention relatesdeep learning-based methodology for developing molecular docking to generate better docking scores.Molecular Docking is a strategy to examine the conformation and orientation to binding site of a specific macromolecule. Recent years have seen a huge adoption of docking techniques both in academic and industrial arenas due to its accuracy and reduced cost. Proposed is a Deep Learning based Molecular Docking system to yield better docking scores. The system uses Quantitative Structure Activity Relationship for systematically eliminating the non-favorable molecules during the iterations of docking.