SYSTEM AND METHOD FOR PREDICTING BINDING AFFINITY OF SMALL MOLECULES TO RNA TARGETS

IITM Technology Available for Licensing

Problem Statement

- In the existing approaches like Computer-Aided Drug Design (CADD) have primarily been focused on the development of scoring functions or models, which can predict the in vitro activity of any given small molecule against a specific target protein or nucleic acid.
- The technical problem, underlying the present invention, may be regarded as the **absence of generic quantitative prediction** models for predicting binding affinity of **RNA targets** of different RNA families with small molecules.
- Hence, said invention provides suitable solution by addressing the issues efficiently.

Technology Category/ Market

Technology: Predicting binding affinity of small molecules to RNA targets;
Industry & Application: Pharmaceutical, Biotechnology, Cellular & Biological Simulation, Drug Discovery & Disease Modelling
Market: The global computational biology market is projected to grow **$31.5Bn** by **2031,** at a **CAGR** of **19.5%** during the forecast period **(2024-31).**

Technology

- Present invention provides a **system** and **method** for **predicting binding affinity** of small molecules to Ribo-Nucleic Acid (**RNA**) targets. (Refer Figs. 1, 2 & 3)
- Said **system** comprises a **memory** & a **processor** wherein the processor is configured to **receive an input** from a user & **predict a binding affinity** of the small molecule to the **RNA target** of the sub-type, using a prediction model.
- In the embodiment, the one/more modules may be communicatively coupled to the processor for performing the functions of the binding affinity predicting system, wherein the modules comprises a receiving module, an RNA feature calculation module, a small molecule feature calculation module, a prediction model generating module, a prediction model, an executing module and other modules.

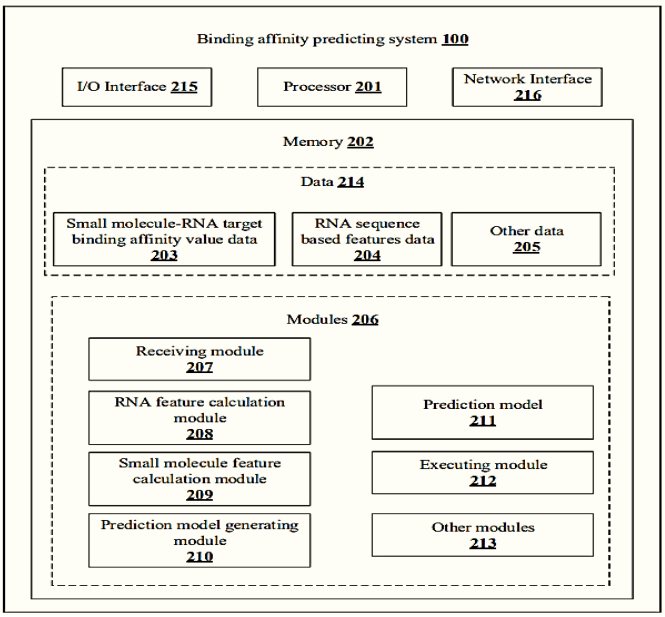

Fig. 1 shown detailed block diagram of a binding affinity predicting system for implementing embodiments

- The prediction model generating module is configured to identify a plurality of non-correlated features from the plurality of RNA sequence-based features & the plurality of small molecule features.

Intellectual Property

IITM IDF Ref. 2554;
Patent Application No. 202341049440

TRL (Technology Readiness Level)

TRL-4, Proof of Concept ready, tested and validated in Laboratory

Research Lab

Prof. Michael Gromiha M;
Dept. of Biotechnology

CONTACT US
Dr. Dara Ajay, Head TTO
Technology Transfer Office,
IPM Cell- IC&SR, IIT Madras

IITM TTO Website:
https://ipm.icsr.in/ipm/

Email: smipm-icsr@icsrpis.iitm.ac.in
sm-marketing@imail.iitm.ac.in
Phone: +91-44-2257 9756/ 9719

Technology (Contd.)

- A method for predicting binding affinity of small molecules to RNA targets, comprising a few steps shown in flow chart depicted in **Fig. 2** herein:

Receiving an input from a user, comprising a sequence of an RNA target, information related to a small molecule and a sub-type of the RNA target

↓

Predicting a binding affinity of the small molecule to the RNA target of the sub-type, using a prediction model

↓

Wherein generating the prediction model comprises:

↓

Obtaining a plurality of RNA sequence based features for a plurality of sub-types of a plurality of RNA targets, and a plurality of small molecule features for a plurality of small molecules

↓

Identifying a plurality of non-correlated features from the plurality of RNA sequence based features and the plurality of small molecule features

↓

Generating a final feature combination from the plurality of non-correlated features for each sub-type of the plurality of sub-types of the plurality of RNA targets based on a quasi-binding affinity of each of the plurality of small molecules with each sub-type of the plurality of sub-types of the plurality of RNA targets, wherein the final feature combination is used to generate the prediction model

Images

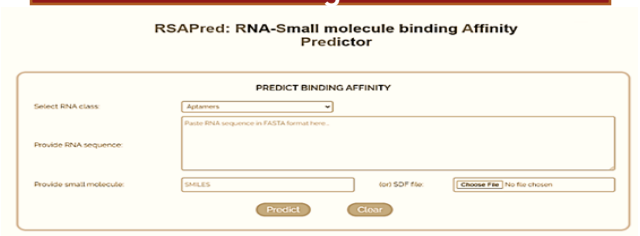

Fig. 3 depicts exemplary web-based tool for implementing embodiments

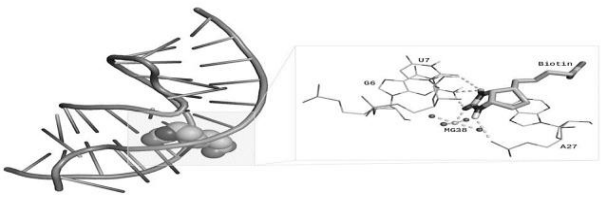

Fig.4 shows a first exemplary interaction in accordance with an embodiment;

RNA subtype	AUROC score	Average precision	Specificity	Sensitivity/Recall	F1-score	MCC
Aptamers	0.97027	0.95724	0.96391	0.97663	0.97209	0.94105
miRNAs	0.96642	0.92525	0.96733	0.96551	0.95522	0.92881
Riboswitches	0.95345	0.92968	0.93607	0.97082	0.95623	0.90833
Viral RNAs	0.98439	0.97949	0.98548	0.98331	0.98520	0.96856

Table 1 depicts performance of the binding affinity prediction models on four classification datasets.

Key Features / Value Proposition

❖ Important Features:

- The system predicts the binding of affinity of novel small molecules to RNA targets from **six RNA subtypes** using **only the RNA sequence** as input.
- The RNA sequence-based features data may be classified into three categories like **oligonucleotide or K-tuple nucleotide composition, pseudo-nucleotide composition & structure composition.**
- The prediction model generating module may identify the **final feature combination** as the feature combination with the **smallest** number of features, offering **optimal** performance, wherein the performance variables may be Pearson correlation coefficient (r) & Mean Absolute Error (MAE).
- Facilitates an **improved performance** of the binding affinity predicting system & also provides a **reduction** in the feature **calculation load** for the binding affinity predicting system. (Refer Fig 4 and Table 1)
- The experimental software model of **RNA–small molecule binding affinity predictor** is shown in Fig. 3.

CONTACT US
Dr. Dara Ajay, Head TTO
Technology Transfer Office,
IPM Cell- IC&SR, IIT Madras

IITM TTO Website:
https://ipm.icsr.in/ipm/

Email: smipm-icsr@icsrpis.iitm.ac.in
sm-marketing@imail.iitm.ac.in
Phone: +91-44-2257 9756/ 9719