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Bio-AIMS Chemoinformatics Web Tools for Proteins

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Abstract: The peptide biological screening represents a difficult task due to the complexity of the amino-acid sequences. One solution is the encoding of the molecular information using complex networks or graphs of the peptides into QSAR-like models in Web tools. Bio-AIMS contains free Web tools on an Artificial Intelligence Model Server in Biosciences: http://bio-aims.udc.es/TargetPred.php. These in silico peptide screening tools are implementing models to predict different protein activities, drug – protein and protein – protein interactions. The inputs are using 3D protein structures or 1D peptide amino acid sequences and the SMILES formulas for drugs, and the classification models are based on Machine Learning techniques. The Web tools are implemented using Python, PHP and XHTML programming languages.

Keywords: molecular information, Machine Learning, protein graphs, Python scripts, QSAR models, Web tools

1. Introduction

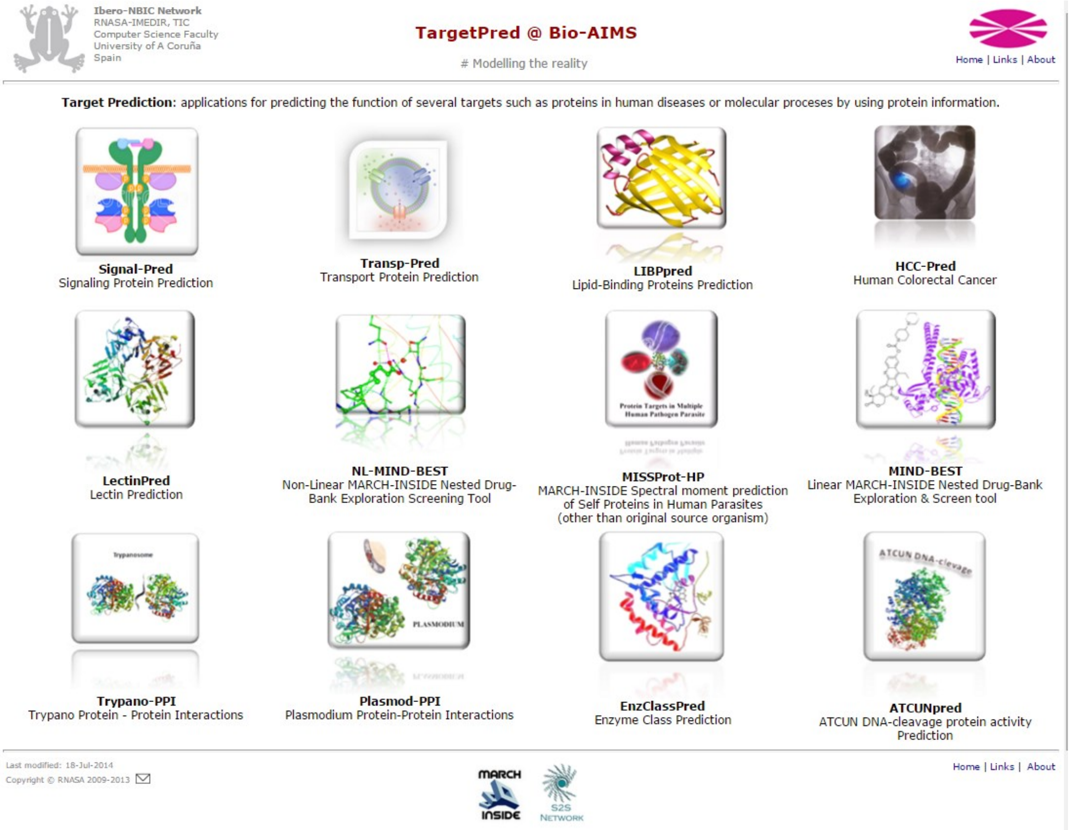
The *in silico* screening methods are very important in Drug Development or proteomics. The theoretical screening is a fast and low cost option to filter the large number of molecules or macromolecules for a specific biological action or chemical property.

These methods are proposing prediction models such as Qualitative Structure-Activity/Property Relationships (QSAR/QPDR), relations between the molecular structure and its activity [1,2]. Extended publications are using small molecule QSAR models. The current collection of QSAR-like models implemented into Web tools are extended the QSAR methodology to macromolecules [3].

2. Results and Discussion

The collection of free Web tools of Target Prediction section of Bio-AIMS server are implementing 12 classifiers (http://bio-aims.udc.es/TargetPred.php, see Figure 1):

- **Signal-Pred**: Signaling Protein Prediction [4]
- **Transp-Pred**: Transport Protein Prediction [5]
- **LIBPpred**: Lipid-Binding Proteins Prediction [6]
- **HCC-Pred**: Human Colorectal Cancer Protein Prediction [7]
- **LectinPred**: Lectin Prediction [8]
- **NL-MIND-BEST**: Non-Linear MARCH-INSIDE Nested Drug-Bank Exploration Screening Tool [9]
- **MISSProt-HP**: MARCH-INSIDE Spectral moment prediction of Self Proteins in Human Parasites (other than original source organism) [10]
- **MIND-BEST**: Linear MARCH-INSIDE Nested Drug-Bank Exploration & Screen tool [11]
- **Trypano-PPI**: Trypano Protein - Protein Interactions [12]
- **Plasmod-PPI**: Plasmodium Protein-Protein Interactions [13]
- **EnzClassPred**: Enzyme Class Prediction [14]
- **ATCUNpred**: ATCUN DNA-cleavage protein activity Prediction [15].



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TargetPred @ Bio-AIMS

Modelling the reality

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Target Prediction: applications for predicting the function of several targets such as proteins in human diseases or molecular proceses by using protein information.

Signal-Pred
Signaling Protein Prediction

Transp-Pred
Transport Protein Prediction

LIBPpred
Lipid-Binding Proteins Prediction

HCC-Pred
Human Colorectal Cancer

LectinPred
Lectin Prediction

NL-MIND-BEST
Non-Linear MARCH-INSIDE Nested Drug-Bank Exploration Screening Tool

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Trypano-PPI
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Figure 1. Bio-AIMS Target Prediction with 12 free Web tools for proteins

3. Materials and Methods

The molecular information was encoded into graph/network molecular descriptors [16]: in the case of proteins/peptides, the nodes are the amino acids and the edges are the peptide bonds and graph specific properties [17-19].

The set of molecular descriptors with the specific protein activities or properties have been used as input for the Machine Learning techniques to obtain the best classifier predictors.

The best protein predictors are implemented into 12 free Web tools as Target Prediction section of Bio-AIMS server: http://bio-aims.udc.es/TargetPred.php.

The inputs of these tools are protein PDB name [20,21], SMILE chemical formulas for drugs or peptide sequences. The tools to calculate the descriptors are MARCH-INSIDE (Python version) [22] and S2SNet – Sequence to Star Network [23,24] (programmed in Python/Biopython [25] The Machine Learning methods [26] have been used from STATISTICA [27], Weka [28] and R [29]. The Web tools were programmed in XHTML [30], PHP [31], Python [25], and R [29].

4. Conclusions

This short communication is presenting a collection of free Web tools for protein prediction at Bio-AIMS. These tools are based on protein descriptors obtained with molecular graphs, Machine Learning methods to search for the best classifier and Python/PHP/XHTML/R programming languages.

This collection is an important contribution to the open science and demonstrate the power of encoding of the molecular information into molecular graph descriptors for proteins/peptides.

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Conflicts of Interest

The authors declare no conflict of interest.

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