SOFTWARE FOR 3D SPECTRAL FINGERPRINT BASED CONSENSUS MODELING USING ORTHOGONAL PLS AND TANIMOTO SIMILARITY KNN TECHNIQUES

Technology Summary

This technology is a software tool for improving molecular modeling. The software addresses data matrices processed in rows instead of columns and the result of these approaches are combined. To process data in rows, the technique uses a measure of similarity known as "Tanimoto Similarity" operating on pairs of objects. The property values of the topmost similar objects are normalized and used as coefficients to predict the property of interest. These predictions can then be used in combination with the predictions obtained by multivariate techniques to improve the quality of the consensus model in comparison to the individual predictions. Since, in the case of multivariate techniques, the information is accessed in columns, while for the similarity-based technique it is accessed in rows, the two types of techniques provide complementary information. Thus, more useful information can be extracted from the same data matrix.

Also contemplated is the use of consensus modeling by letting two algorithms (PLS and KNN) operate on descriptor matrices of different size. If each of these matrices is processed by a different model building algorithm and a consensus model between two or more such individual models is built, the resulting model would benefit from both: i) the partial orthogonality of the modeling techniques and ii) the complementarity of the information contained in 3D-SDAR matrices of different granularity.

Potential Commercial Applications

- Drug Design
- Drug Development

Competitive Advantages

- Matrix processing of molecules of biological interest
- High Fit-Activity Prediction capacity

Development Stage: Research Tool, Software

Inventors: Svetoslav Slavov, Jon Wilkes, Rick Beger, Dan Buzatu, Bruce Pearce

Publications:

- Slavov SH, et al. ^{13}C NMR-distance matrix descriptors: optimal abstract 3D space granularity for predicting estrogen binding. J Chem Inform Model. 2012 Jul 23;52(7):1845-64. PMID: 22920720
- Slavov SH, et al. Complementary PLS and KNN algorithms for improved 3D-QSDAR consensus modeling of AhR binding. J Cheminform. 2013, 5: 47 - 62. PMID: 24257141
- Stoyanova-Slavova IB, et al. PLS and KNN algorithms for improved 3D-QSDAR consensus modeling of acute toxicity. Accepted for publication in Environ Toxicol Chem. 2014 Jun;33(6):1271-82. PMID: 24464801

Product Area: Research tool, software, bioinformatics, modeling

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Licensing Contact:
Ken Millburne, J.D.
FDA Technology Transfer Program
Email: FDAInventionlicensing@fda.hhs.gov
Phone: 240-402-2245