Transform-MinER and the biosynthetic chemical design space

Leidi Hernández
lhsuarez96@gmail.com

Department of Pharmacology, Faculty of Medicine, University of the Basque Country UPV/EHU, 48940, Leioa, Basque Country, Spain

Graphical Abstract (mandatory)

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For the study of enzymatic designs and directed evolution projects, a relevant program would be
Transform-MinER. In the article Exploring the space of the biosynthetic chemical design with Transorm-MinER, it is explained that this by means of molecular transformations in enzymatic reactions, allows to explore the chemical space by searching for a starting point. With the use of chemoinformatic fingerprints, it searches for possible reaction centers in the source substrate and identifies those in environments similar to those of the natives. It uses two types of search for enzymatic reactions in similar substrates and for enzymatic reactions that link the source and the target with the sending of a target molecule (molecule search and route search, respectively). Through the KEEG database, which is nothing more than a collection of database of genomes and metabolic pathways and de novo enzymatic reaction data, its performance is determined, with a 90% success considered optimal. On the other hand, the article Transform - MinER: transforming molecules into enzymatic reactions, reaffirms the fact that said program facilitates the identification of initial enzymes in an investigation, since it finds the most similar native enzymatic reactions emphasizing those of greater interest to the researcher.

KEYWORDS: chemoinformatics; data-mining; enzyme design.


https://www.ncbi.nlm.nih.gov/pmc/articles/PMC102409/