World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:16, No:03, 2022

Employing a Knime-based and Open-source Tools to Identify AMI and VER Metabolites from UPLC-MS Data

Authors : Nouf Alourfi

Abstract : This study examines the metabolism of amitriptyline (AMI) and verapamil (VER) using a KNIME-based method. KNIME improved workflow is an open-source data-analytics platform that integrates a number of open-source metabolomics tools such as CFMID and MetFrag to provide standard data visualisations, predict candidate metabolites, assess them against experimental data, and produce reports on identified metabolites. The use of this workflow is demonstrated by employing three types of liver microsomes (human, rat, and Guinea pig) to study the in vitro metabolism of the two drugs (AMI and VER). This workflow is used to create and treat UPLC-MS (Orbitrap) data. The formulas and structures of these drugs' metabolites can be assigned automatically. The key metabolic routes for amitriptyline are hydroxylation, N-dealkylation, N-oxidation, and conjugation, while N-demethylation, O-demethylation and N-dealkylation, and conjugation are the primary metabolic routes for verapamil. The identified metabolites are compatible to the published, clarifying the solidity of the workflow technique and the usage of computational tools like KNIME in supporting the integration and interoperability of emerging novel software packages in the metabolomics area.

Keywords : KNIME, CFMID, MetFrag, Data Analysis, Metabolomics
Conference Title : ICCCMOEA 2022 : International Conference on Computational Chemistry, Modelling and Engineering Applications
Conference Location : Madrid, Spain
Conference Dates : March 21-22, 2022

Open Science Index, Chemical and Molecular Engineering Vol:16, No:03, 2022 publications.waset.org/abstracts/147907.pdf