

CanGraph: a python utility to study and analyse cancer-associated metabolites using knowledge graphs

Wednesday, 21 September 2022 12:48 (6 minutes)

Research on cancer, one of the most lethal diseases in the world today, is an expensive, complex process, usually carried out manually in laboratories. In this publication, we present CanGraph, a software solution that allows its users to annotate and interpret unknown metabolites by making use of five pre-existing databases (HMDB, SMPDB, DrugBank, ExposomeExplorer and Wikidata) and five search criteria (InChI, InChIKey, Structural Similarity, HMDB_ID, Name and ChEBI ID), resulting in an output database in GraphML format containing the associations to the different metabolic pathways, tissues and organisms to which these molecules may belong. Although it still presents problems, such as the long processing time, we hope that this program will be useful in automating the search for potential relationships between compounds and various diseases (specially cancer, as is the mission of International Agency for Research on Cancer (IARC), the Institution where this project has been carried out), with a view towards generating a web service that will make this program, and all its knowledge, available to the scientific community at large.

Primary author: MARCOS LOPEZ, Pablo (IARC)

Co-authors: AMARA, Adam (IARC); POVEDA VILLALÓN, María (Universidad Politécnica de Madrid)

Presenter: MARCOS LOPEZ, Pablo (IARC)

Session Classification: Lightning poster presentation