Connecting the worlds of metabolomics databases

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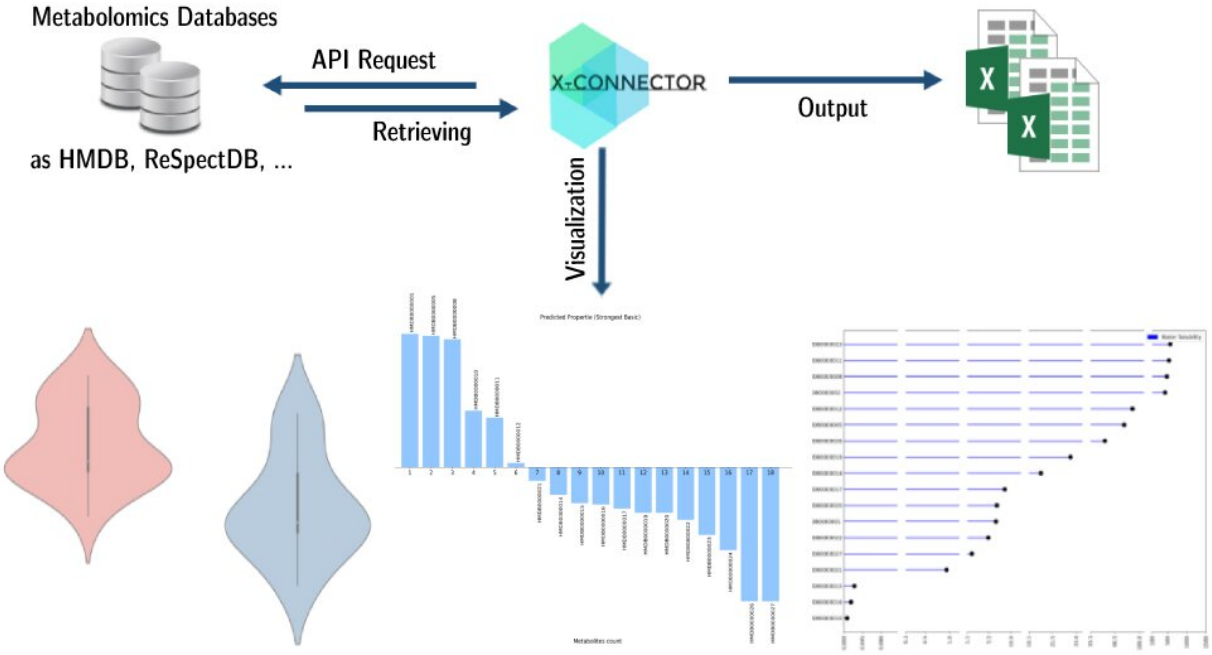

Xconnector software. Credit: Proteomics and Metabolomics research program, Basic research department, Children's Cancer Hospital 57357 (CCHE-57357).

Collecting the data is a critical step for any research project to kick off. For biomedical scientists, this means delving into petabytes of data scattered into hundreds of public or private databases.

"This process could be overwhelming and time-consuming for many

researchers," says Ali Mostafa, a bioinformatician in CCHE 57357 proteomics and metabolomics research program, and the first author on a paper recently published in the *Journal Of Proteomics* describing a new software package (Xconnector) that easily retrieves and visualizes metabolomics information from multiple databases.

Metabolomics is broadly defined as the large-scale study of metabolism substrates and products within cells, tissues or body fluids.

"Unlike genomics approaches that examine individual variability, or transcriptomics that detect the actual active genes, metabolomics is more dynamic and could capture temporal and tissue-specific changes in response to diseases or treatment. That's why it's becoming more promising for precision medicine approaches," says Sameh Magdeldin head of proteomics and metabolomics research program and the corresponding author on the paper.

The growing interest in metabolomics is reflected in the tens of public repositories that contain a huge diversity of metabolites information.

However, each database has its unique format and data, which makes the manual collection of big data required for performing a high throughput analysis a very tedious and inefficient process.

"Each metabolomics database is in its own world, connecting those worlds into an accessible format for researchers with publishable explanatory graphs is at the core of the newly developed Xconnecter software," Ali said.

Xconnector can access and retrieve data from several large databases including but not limited to Human Metabolome Database (HMDB), Livestock Metabolome Database (LMDB), Yeast Metabolome Database (YMDB), Toxin and Toxin Target Database (T3DB), and Blood

Exposome Database (BEDB).

Moreover, The software can visualize the retrieved data, which would assist the researchers in choosing the optimum analysis strategy.

It's also free to download and doesn't require any prior coding skills, Ali Said.

Previously, the same team has designed a powerful protein data retrieval tool called UniprotR, which was downloaded more than 18,000 times. In the future, The team intends to update these tools with more functionalities and to connect them with additional databases.

"We believe data gathering tools like Xconnector will expedite research efforts aiming to uncover novel biomarkers, and unravel unknown biological pathways," Magdeldin Says.

More information: Anwar A, et al. Xconnector: Retrieving and visualizing metabolites and pathways information from various database sources. *J Proteomics*. 2021 Jun 7:104302. DOI: 10.1016/j.jprot.2021.104302. Epub ahead of print. PMID: 34111608.

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