Mira Syahfriena Binti Amir Rawa
May 28, 2019

Journal Club no. 830

A Cheminformatics Approach to Characterize Metabolomes In Stable-Isotope-Labeled Organisms

Hiroshi Tsugawa*, Ryo Nakabayashi, Tetsuya Mori, Yutaka Yamada, Mikiko Takahashi, Amit Rai, Ryosuke Sugiyama, Hiroyuki Yamamoto, Taiki Nakaya, Mami Yamazaki, Rik Kooke, Johanna A. Bac-Molenaar, Nihal Oztolan-Erol, Joost J. B. Keurentjes, Masanori Arita and Kazuki Saito*

Nature Methods, Vol. 16, 295-298, April 2019

As structure determination has become essential in metabolomics and natural products studies, advances in metabolomic technologies are essential for high-throughput screening of natural products. Generally, conventional techniques of structure elucidation involve LC-MS and NMR. It requires isolation of a single metabolite and comparison with the available databases to determine the compound. This paper discussed online methods in characterizing untargeted metabolomes that analyzes mass fragmentation of ions (LC-MS/MS) and ^{13}C-labeled and non-labeled plants to determine the carbon numbers and classify unknown molecules.

Abstract

We report a computational approach (implemented in MS-DIAL 3.0; http://prime.psc.riken.jp/) for metabolite structure characterization using fully ^{13}C-labeled and non-labeled plants and LC–MS/MS. Our approach facilitates carbon number determination and metabolite classification for unknown molecules. Applying our method to 31 tissues from 12 plant species, we assigned 1,092 structures and 344 formulae to 3,604 carbon-determined metabolite ions, 69 of which were found to represent structures currently not listed in metabolome databases.