conferenceseries.com

Kieu Oanh T Nguyen et al., Metabolomics 2017, 7:2(Suppl)
http://dx.doi.org/10.4172/2153-0769-C1-037

A computed biochemical conversion network revealed a broad spectrum of hydroxycinnamic acid ester conjugates of glucaric acid in *Isatis tinctoria* leaves

Kieu Oanh T Nguyen[1], Eric Gontier[2] and Rebecca Dauwe[2]
[1]University of Science and Technology of Hanoi, Vietnam
[2]University of Picardy Jules Verne, France

Isatis tinctoria is a plant species belonging to the Brassicaceae family that is known as an ancient source of indigo dye and as a medicinal plant with high industrial potential. Although a large comprehensive metabolite profiling of the bio-active dried leaf extracts has been reported, metabolite profiling of *Isatis* fresh leaves focused up to today on glucosinolates and flavonoids. We profiled here the methanol extracts of *I. tinctoria* fresh leaf extracts in an untargeted way and aimed especially to detect as yet unidentified compounds. Therefore, an algorithm was adopted in which liquid chromatography-mass spectrometry profiles are searched for pairs of peaks that have mass and retention time differences corresponding with those of substrates and products from well-known biochemical conversions. We then concatenated these peak pairs into a network where the nodes represent metabolites and edges represent biochemical conversions. Starting from known network nodes, following the edges of the network allowed the characterization of adjacent network nodes, leading to their structure. This high-throughput cheminformatics procedure allowed the characterization of the structures of a wide spectrum of hydroxycinnamic acid esters. Besides the sinapate esters of malate, glucose and gentiobiose, which are typical for brassicaceous plants, these conjugates comprised a large variety of glucaric acid esters which have not been reported in plants before. This untargeted approach suggests the existence of an as yet unknown acyltransferase activity in *Isatis tinctoria* rosette leaves.

Biography

Kieu Oanh T Nguyen has research interests on small molecule measurements and metabolomics in plants. She is also interested to apply metabolomics approach in natural product drug discovery (dereplication, chemotaxonomy, metabolic engineering). Her expertise is in the development of screening pipelines for small molecule extraction, isolation and derivatization where necessary, chromatographic separation (liquid and gas chromatography) and detection including mass spectrometry.

nguyen-thi-kieu.oanh@usth.edu.vn

Notes: