Aiko Barsch, J Comput Sci Syst Biol, 5:1
doi: http://dx.doi.org/10.4172/0974-7230.S1.12

OMICS Group Conferences
Accelerating Scientific Discovery

International Conference and Exhibition on
Metabolomics & Systems Biology

20-22 February 2012 San Francisco Airport Marriott Waterfront, USA

Structure elucidation and confirmation in plant metabolomics: Novel approaches exemplified with acyclic diterpene gylcosides

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Presently, the key bottleneck of (plant) metabolomics is structural confirmation and elucidation of secondary metabolites. *Nicotiana attenuata* is a well-established model system to monitor plant-herbivore interactions with metabolomics being a novel approach to investigate the underlying biology [1]. 17-Hydroxygeranyllinallool diterpene glycosides (HGL-DTGs) are abundant direct defense compounds with their mode of action being largely unknown [1-3]. New acyclic HGL-DTGs were characterized using MS and NMR after extraction of several hundred grams of raw plant material [2, 3]. Such scale is not compatible to the analytical scope of metabolomics. Here, we present novel solutions facilitating the identification and fast dereplication process of natural products when mass spectral libraries are not yet available and the sample amount is limited.

Plant samples were prepared as described previously [1]. Chromatographic separation was carried out using an UHPLC system combined with ultra high resolution (UHR) Q-TOF MS detection. Selected plant samples were fractionated. Peaks enriched in HGL-DTGs were subjected to detailed fragmentation studies by means of direct infusion measurements.

The dereplication of HGL-DTGs is rendered difficult by the large number of in-source fragments and adduct formation, and their molecular weight of 800-1000m/z. Novel algorithms were applied for deconvolution of LC-MS chromatograms by correlation analysis to safely determine the molecular ion in the presence of adducts and in-source CID fragments. Molecular formula determination was carried out by combined evaluation of mass accuracy, isotopic patterns, adduct and fragment information. The diagnostic fragments for the HGL-DTG backbone and successive sugar units, such as $[M+H]^+$ = 271.2420m/z = $C_{20}H_{31}^+$ and 417.2999m/z = $C_{26}H_{41}O_4^+$ enabled the rapid identification of the entire compound family, which is subsequently characterized in more detail. For this, the fragmentation results have been combined with the structural information to visualize the interpretation. Simultaneously the necessary validation prior submission to a mass spectral library is achieved.