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Nano-Liquid chromatography coupled MALDI MS/MS based quantitative cancer metabolomics

Swarnendu Bag
Tata Medical Center, India

Tumour cells follow aberrant metabolic process for its survival and to escape from immune attack. Quantitative metabolomics is very crucial to understand the altered cancer micro-environment for targeted cancer theranostics. In this context, high-throughput separation and quantification of metabolites from clinical samples is an essential domain. Matrix Assisted Laser Desorption Ionization Mass Spectrometry (MALDI-MS), a gold standard technique for metabolite identifications, suffers from limitations in quantitation. In present work, a novel approach having nano-LC-MALDI MS/MS interface for separation, identification and label free quantifications of the metabolites from bio-samples has been evaluated. Metabolites extracted from cancer biopsies were separated and subsequently eluted as fraction spots on MALDI target plate. Introducing a novel parameter, % AAUC, quantification of metabolites isolated from cancer biopsies was explored. This comparative quantification is only possible with multiple AUCs of a particular metabolite obtained from this nano-LC-MALDI-MS. Selected metabolite peaks were analyzed through MS/MS fragmentation tool. This novel method was validated using known concentrations of an internal standard (thiourea). The novel quantification method revealed a significant change in expression of lipid metabotypes like phosphatidyl-choline, triglyceride, cytidine-diphosphate-diacylglycerol and phosphatidylinositol bisphosphate representing de-regulated lipid metabolism in oral cancer.