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PALMS: Parallel targeted/untargeted metabolome screening platform

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The human body contains about 10 microbes per each human cell if you do not consider red blood cells which are lacking DNA. This means microbes significantly impact the chemistry in and on our body. Despite the role of microbial chemistry on human health, we know very little about its chemistry, let alone quantitatively. One of the analytical methods that are sensitive enough to measure microbial chemistry can be mass spectroscopy (MS). Here we introduce PALMS platform that is capable of analyzing full sample profile using high accuracy Orbitrap instrument and quantify set of targeted metabolites using triple quadrupole in a single LC run. Several hundred of fecal swabs samples from the American Gut project were tested and then people were swabbed at several hundred locations for the creation of 3D quantitative maps. The system setup comprises of triple quadrupole (qqq) and Orbitrap mass spectrometers connected in parallel to a single UHPLC system. Liquid connection was split into equal ratio and directed into two MS which are equipped with identical HESI ion sources; tubing length maintained equal in order to avoid any retention time (RT) differences between two MS. The data acquisition was triggered by UHPLC system by mean of contact closure signal that is sent to both MS simultaneously. Data captured by Q Exactive recorder in untargeted profiling mode with high resolution while quantitative data on defined targets were acquired by TSQ. We first evaluated our system by screening of several hundreds of fecal swabs extracts received from American Gut project. For targeted quantification we used mix of 200 standards containing microbial primary and secondary metabolites. We evaluated a distribution of the standards in fecal samples by constructing a calibration curve with triple quadrupole data. Our results showed that even in such high background as fecal matter we can quantify metabolites with relatively low error rate. By feeding mass list to triple quadrupole we managed to achieve pictogram sensitivity at the same time acquiring a full molecular profile using Orbitrap. By analyzing untargeted data we were able to putatively identify thousands of molecules using molecular networking while quantification was performed for selected microbial metabolites. Because in molecular networking structurally similar molecules clustered together we were able to relatively quantify analogs of the standards by extrapolating their concentrations. We then used the platform for screening the microbial metabolites reside on human body. We constructed 3D chemical composition maps of human skin surface. Highly accurate, untargeted data allowed for identification of some key microbial metabolites that are distributed on the skin in the specific locations such as armpit and groin area. We then relatively quantified the metabolites as some of our standards clustered with molecules of interest, which concentration was accurately measured by triple quadrupole. Determining the quantitative information for key microbial metabolites grant us the possibility to calculate the amount of the microbial cells that are primary producers and potentially assess the impact of them on our health.

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Sub-2 µm C18 bound silica monolith particles as HPLC stationary phase of high separation efficiency

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Sub-2 µm porous silica monolith particles have been prepared successfully by sol-gel process followed by grinding and calcinations at 550 oC. The particles were derivatized with a C18 ligand followed by end-capping with a mixture of hexamethyldisilazane (HMDS) and trimethylchlorosilane (TMCS). The resultant phase was packed in glass lined stainless steel microcolumn is much better than that of commercial C-18 phase. This phase has shown some encouraging possibility for fast analysis when packed in a short column. This study offers a promising vision towards commercialization of chromatographic phases based on silica monolith particles.

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