

July 05-07, 2018  
Berlin, GermanyZhang Jinlan, Arch Chem Res 2018, Volume 2  
DOI: 10.21767/2572-4657-C3-008

## AN APPROACH FOR UNTARGET TO TARGET METABOLOMICS FOR DIFFERENT BIO-SAMPLES

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A novel approach known as “database based dynamic target metabolomics”, from untargeted recognition and identification to targeted quantification for metabolites in bio-fluid samples on the basis of metabolomic database were developed. The RP-UHPLC/MS and HILIC-UHPLC/MS system were performed for untargeted lipid and polar metabolite profiling, respectively. Metabolite peak features in RP and HILIC systems were assigned by molecular feature extract to remove interference from other fragment ions. HRMS/MS data of assigned metabolites were processed by the Lipid Maps database to identify the lipid compounds and the METLIN QTOF MS/MS database and PCDL database for the polar metabolites in different biological samples. The identified metabolites both lipid and polar compounds were assigned to generate the targeted lists for quantification, and the in-home PCDL HRMSMS database of targeted metabolites for different bio-sample was established. This approach is suitable for modern metabolomic research which takes the advantages of the untargeted recognition and identification ability and the targeted accuracy quantification, with the dynamic and automatic characterization.

### Biography

Zhang Jinlan is a professor of pharmaceutical analysis of Institute of Materia Medica, Chinese Academy of Medical Sciences. Dr. Zhang has more than 90 publications and received several awards. She was chosen to be in the 2009 New Century talent plan by the Chinese Ministry of Education. Prof. Zhang also serves numerous titles such as Committee members of Chinese MS Society (CMMS) Committee for Organics, Authorized Laboratory Auditor for the World Anti-Doping Agency (WADA), etc. Her research interests include method development and standardization for active ingredients in herbal medicine, DMPKT of new drugs, and metabolomics based mass spectrometry. Her research interests are Method development and standardization for active ingredients in herbal medicine, Metabolism of herbal medicine and DMPKT of new drugs, Metabolomics based mass spectrometry.

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