Holistic Integrative Pharmacology

2018 Harbin Summit of Chinmedomics and Drug Metabolism

冰城夏都哈尔滨欢迎您

中国 哈尔滨

2018 年 6 月

整合药理学：2018 哈尔滨中医方证代谢组学与药物代谢峰会

Holistic Integrative Pharmacology: 2018 Harbin Summit of Chinmedomics and Drug Metabolism

（第一轮通知）

大会主题： 精准代谢分析助力中药（药物）精准研究

Precision-Metabolic Assay Promotes TCM (Drugs) Innovation

主办单位： 国家中医方证代谢组学研究中心

中－美中医方证代谢组学技术合作中心

海军军医大学

上海交通大学

承办单位： 黑龙江中医药大学，西南濒危药材资源开发国家工程实验室

协办单位： 沃特世（中国）有限公司等

合作媒体： 世界中医药杂志（WJTCM），Acta Pharmaceutica Sinica B 等

华旗饭店 中国 哈尔滨（具体地点详见第二轮通知）

2018 年 6 月 22-24 日

会议简介（CONFERENCE INTRODUCTION）

人类步入二十一世纪，聚焦人类健康与疾病谱多尺度与多维度的复杂性，经典的细胞与分子生物学研究方法已经无法满足快速捕获各类疾病的分子表型（Molecular Phenotype），无法做到对疾病发生发展过程中的动态分子特征谱（Molecular Phenome）进行全景式描述，无法精准完成复杂疾病从基因表型到功能表型的快速对接与网络化整合，进而错失对疾病病源机理的系统定性描述和定量表征的最佳机会，最终导致疾病的滞后诊断和最佳治疗时机和方案的制定与实施。

最近 20 年，快速发展的定位于生命体生理与病理过程的全局分子变化的系统生物学方法，对上述科学挑战正在给出全新的组学解决方案，如基因组、转录组和蛋白组技术。这些技术已经在人类健康、疾病和药物研究领域取得了显著的进步，实现从诊断、治疗到新药发现等多领域的实质性突破。这些技术在中国、乃至世界范围内均得到快速发展和应用。 然而，这些新技术主要集中于大分子层面对于生命体生理和病理的描述与表征，尚缺乏靶向生命体分子信息流最后一环，小分子代谢产物的表型与功能的系统认识，而无论是高等生物的人，还是动物，植物或低等微生物，小分子代谢均提供其细胞生长、增值、分化和表达功能所必需的能量、营养成分和生物化学基质环境。因此从小分子代谢产物的表达与修饰角度有助于我们更好的认识生命体的生理与病理过程，助推精准诊断、精准治疗和精准药物开发。暨代谢组学的问世，为我们研究与生命过程代谢相关的科学问题的解决提供了最有效的精准分析方法和策略。

中医药作为中国送给世界的礼物，在几千年的人类繁衍生息与发展过程中，以其独特的医学理论，诊疗方法和用药体系，越来越被国际医学界所重视，其在

多种复杂性疾病诊疗和保障群体健康方面发挥着不可替代的作用。2017 年中国中医药法正式颁布实施，中医药迎来历史最好的发展时期，中国政府将从顶层设计，政策导向，研究资源优化配置，以及现代化和国际化发展战略层面全面护航中医药在全世界范围内的更好更快发展，整体提升中医药服务人类健康的应用水平，以其全新的科学面貌造福世界人民。然而中医药是一个复杂的学科体系，既有理论层面的多维不确定性，又有中药固有化学物质组成的复杂性。目前，其现代化发展与实践应用仍面临巨大挑战，如药效物质基础的辨识，作用机理阐明，有效成分和毒性成分的体内代谢特征与命运，配伍规律，品质一致性评价等。然而中药资源作为现代药物发现与开发不可或缺的重要来源，学界已经达成共识，基于代谢组学策略的精准代谢（药物代谢）分析，或将系统性解决上述瓶颈性关键科学问题，加快实现代创新药物的精准研究与开发。

鉴于代谢组学从系统代谢角度精准解析药物小分子与机体代谢分子复杂作用过程的实践潜力，以及考虑到药物代谢研究策略在新时期天然源小分子药物发现和中药的现代研究等方面的技术优势，**特邀请您参加国家中医方证代谢组学研究中心，中－美中医方证代谢组学技术合作中心，海军军医大学和上海交通大学共同主办的整合药理学：2018 哈尔滨中医方证代谢组学与药物代谢峰会。本次会议拟邀请国内外代谢组学、药理学、药物代谢、精准医学、中医药和毒理学领域的顶尖科学家，2018 年六月，齐聚夏都哈尔滨，共同探讨如何整合全球最优势的智力和学术资源，实现从精准代谢分析到精准中药（药物）研究的实质性突破，升级中医方证代谢组学与现代药物代谢分析策略，更快更好推动未来创新药物发现与开发，实现临床复杂疾病治疗的精准用药，全面提升全人类健康水平。**

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口头报告和海报英文摘要 (ABSTRACTS)

现面向国内外同行征集口头报告（Oral Presentation）和海报 (Poster) 英文摘要。

征集主题如下：

代谢组学新技术新方法（Innovative Methods for Metabolomics Assay）

中医药代谢组学（Metabolomics for Chinese Medicine, Chinmedomics）

药物代谢组学 （Pharmacometabolomics）

药物分析与代谢 (Drug Analysis and Metabolism)

系统药理学 (Systems Pharmacology)

药物代谢动力学/毒代动力学 (Pharmacokinetics/Toxicokinetics)

中药/药物质量评价 (Quality Analysis of Chinese Materia Medica/Drugs)

生命分析化学 (Bioanalytical Chemistry)

生物质谱与组学 (Biological Mass Spectrometry and Omics)

口头报告和海报摘要具体要求与格式详见附件 1-2，口头报告申请者另附上报告者英文简介(Short-Bio)，具体格式与模版详见附件 3，另附会议回执见附件 4。

稿件投递邮箱：chinmedomics2018@163.com； **投稿截止日期**：2018 年 5 月 31 日

注册费标准及汇款方式（REGISTRATION AND FEE）

5 月 1 日前 1200 元人民币，之后和现场交费 1600 元人民币，学生参会注册费 800 元人民币（参会时请出示学生证），汇款时注明 Chinmedomics2018 注册费＋汇款人全名。特邀专家会议费由主办方承担。

汇款信息如下

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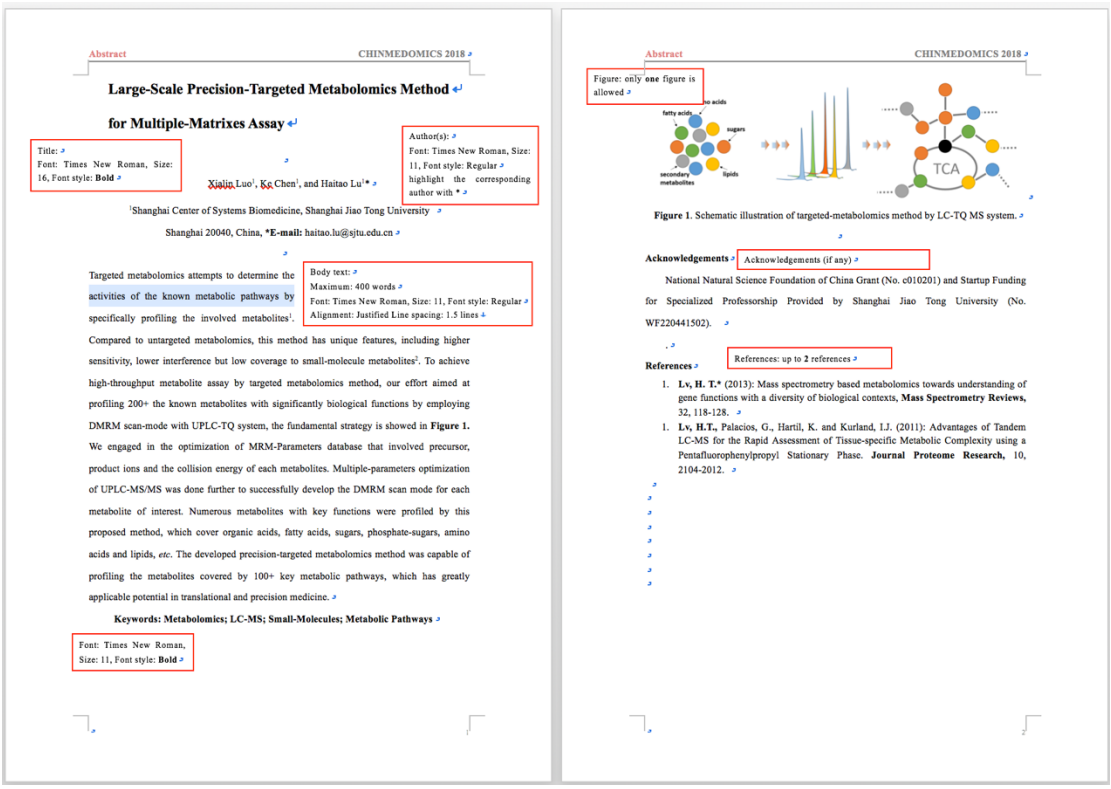
Supplementary File 1

Abstract format shall be as the example here,



Abstract CHINMEDOMICS 2018

Large-Scale Precision-Targeted Metabolomics Method for Multiple-Matrixes Assay

Title: Font: Times New Roman, Size: 16, Font style: **Bold**

Xialin Luo[1], Ke Chen[1], and Haitao Lu[1]*

Author(s): Font: Times New Roman, Size: 11, Font style: Regular highlight the corresponding author with *

[1]Shanghai Center of Systems Biomedicine, Shanghai Jiao Tong University

Shanghai 20040, China, ***E-mail:** haitao.lu@sjtu.edu.cn

Targeted metabolomics attempts to determine the activities of the known metabolic pathways by specifically profiling the involved metabolites[1]. Compared to untargeted metabolomics, this method has unique features, including higher sensitivity, lower interference but low coverage to small-molecule metabolites[2]. To achieve high-throughput metabolite assay by targeted metabolomics method, our effort aimed at profiling 200+ the known metabolites with significantly biological functions by employing DMRM scan-mode with UPLC-TQ system, the fundamental strategy is showed in **Figure 1.** We engaged in the optimization of MRM-Parameters database that involved precursor, product ions and the collision energy of each metabolites. Multiple-parameters optimization of UPLC-MS/MS was done further to successfully develop the DMRM scan mode for each metabolite of interest. Numerous metabolites with key functions were profiled by this proposed method, which cover organic acids, fatty acids, sugars, phosphate-sugars, amino acids and lipids, *etc*. The developed precision-targeted metabolomics method was capable of profiling the metabolites covered by 100+ key metabolic pathways, which has greatly applicable potential in translational and precision medicine.

Body text: Maximum: 400 words Font: Times New Roman, Size: 11, Font style: Regular Alignment: Justified Line spacing: 1.5 lines

Keywords: Metabolomics; LC-MS; Small-Molecules; Metabolic Pathways

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Abstract CHINMEDOMICS 2018

Figure: only **one** figure is allowed

Figure 1. Schematic illustration of targeted-metabolomics method by LC-TQ MS system.

Acknowledgements Acknowledgements (if any)

National Natural Science Foundation of China Grant (No. c010201) and Startup Funding for Specialized Professorship Provided by Shanghai Jiao Tong University (No. WF220441502).

References: up to **2** references

References

1. **Lv, H. T.*** (2013): Mass spectrometry based metabolomics towards understanding of gene functions with a diversity of biological contexts, **Mass Spectrometry Reviews,** 32, 118-128.
1. **Lv, H.T.,** Palacios, G., Hartil, K. and Kurland, I.J. (2011): Advantages of Tandem LC-MS for the Rapid Assessment of Tissue-specific Metabolic Complexity using a Pentafluorophenylpropyl Stationary Phase. **Journal Proteome Research,** 10, 2104-2012.

Supplementary File 2

Poster Size in 42cm ×57cm as the example here,

Metabolic Reprogramming Triggered Biofilm Formation

Rui Guo[1], Xialin Luo[1], Xin Xu[1], Ke Chen[1] and Haitao Lu[1]*

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INTRODUCTION

Urinary Tract Infection (UTI) is a prevalent infectious disease worldwide and pathogenic *E. coli* (UPEC) accounts for approximate 85% clinical cases (1). Previous studies confirmed the biofilm formation contributes significantly to the virulence of UPEC strains, and associated antibiotic resistance (2, 3). Our data has found that the mechanistic link between pathogenicity of *Escherichia coli* and the metabolic modification (4). This study was designed to identify the key small-molecule metabolites that have the capacity to drive biofilm formation via comparing the metabolic differences between biofilm and planktonic cells of UPEC. Then we combined the distinguished molecules with functional studies to clarify the mechanisms to metabolic reprogramming of biofilm formation, which is supposed to provide new hints for biofilm clearance.

METHODS

Firstly, we globally profiled the metabolome of biofilm and planktonic cells of wild type UTI89 by using UPLC/QTOF MS. Secondly, multivariate statistical analysis were performed to analyze the differential metabolome between biofilm and planktonic cells and identify the differential metabolites. Thirdly, modified metabolic pathways involving these key molecules were mapped to annotate the metabolic mechanism of biofilm formation from metabolic perspective.

RESULTS

Distinct changes with morphology and intracellular microstructure have been visualized (**Figure 1**), and global metabolome were shifted remarkably during biofilm formation of UPEC (**Figure 2**), the key metabolites were profiled whose biosynthetic differentiation can significantly distinguish biofilm and planktonic cells (**Figure 3**). At last, mostly affected metabolic pathways were annotated to phenotype biofilm formation (**Figure 4**).

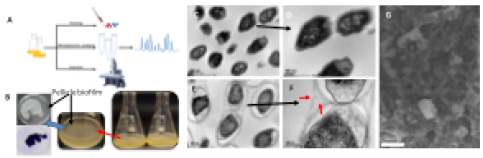

Figure 1. Morphology and intracellular microstructure modification during the biofilm formation.

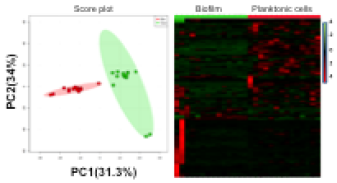

Figure 2. The Global metabolome was shifted markedly during biofilm formation.

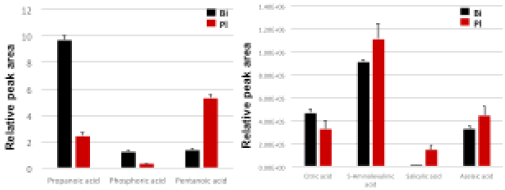

Figure 3. Key metabolites were identified whose level changes can significantly distinguish the biofilm and planktonic cells.

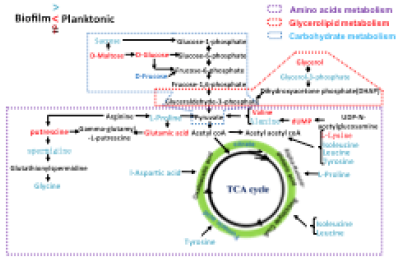

Figure 4. The modified metabolic pathways with biofilm formation

CONCLUSION

Our study suggested metabolic reprogramming might trigger the biofilm formation of UPEC, and functional experiments will be required further to validate this metabolic discovery.

REFERENCES

(1) Ferrieres L, Hancock V, Klemm P. Specific selection for virulent urinary tract infectious *Escherichia coli* strains during catheter-associated biofilm formation. FEMS Immunol Med Microbiol, 2007, 51: 212-9.

(2) Romling U, Balsalobre C. Biofilm infections, their resilience to therapy and innovative treatment strategies. J Intern Med, 2012, 272: 541-61.

(3) Hannan TJ, Totsika M, Mansfield KJ, Moore KH, Schembri MA, Hultgren SJ. Host-pathogen checkpoints and population bottlenecks in persistent and intracellular uropathogenic *Escherichia coli* bladder infection. FEMS Microbiol Rev, 2012, 36: 616–48.

(4) L Yan, W Nie, and H Lv. Metabolic phenotyping of the *Yersinia* high-pathogenicity island that regulates central carbon metabolism. Analyst, 2015, 140: 3356-61.

ACKNOWLEDGEMENTS

National Natural Science Foundation of China Grant (No. c010201) and Startup Funding for Specialized Professorship Provided by Shanghai Jiao Tong University (No. WF220441502).

Supplementary File 3

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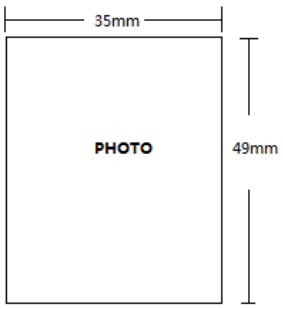

Haitao-Tao Lu, Ph.D.

Faculty Director & Professor
Laboratory for Functional Metabolomics Science
Shanghai Center for Systems Biomedicine
Shanghai Jiao Tong University
Shanghai, China

Please provide us electronic photo with size 35mm*49mm (width*length)

Dr. Haitao Lu is a Professor/Principal Investigator at Shanghai Center for Systems Biomedicine, Shanghai Jiao Tong University (Shanghai, China). He is a high-profile young scientist with over 10 years' research, teaching and management experience in the fields of functional metabolomics, microbial metabolism and systems biology of Chinese Herbal Medicine. Dr. Lu was conferred a B.SC degree in 2004 and a PhD degree in 2009 by Heilongjiang University of Chinese Medicine in China. After Postdoctoral Trainings in Albert Einstein College of Medicine, Washington University School of Medicine, MIT in USA from 2009 to 2012, he took over a professor position in Chongqing University in China until December 2015, where he was in charge of Laboratory of Functional Omics and Innovative Chinese Medicine. Since December 2015, He started to lead the development and innovation of The Laboratory for Functional Metabolomics Science in SJTU. In addition, he was granted with the prestigious Vice Chancellor's Research Fellowship by QUT in July 2013. He has authored and co-authored 40 peer reviewed papers in many high-profile journals, such as Mass Spectrometry Reviews, Journal of Proteome Research, Molecular and Cellular Proteomics, etc. as well as 30+ conference publications. In recent five years, He successfully secured three national competitive grants and several prestigious fellowships from different Funding Agencies and Universities in China, USA and Australia, with total funding is more than US $ 1 million. He is also acting as an academic membership for the Editorial Board of several peer-reviewed journals, Scientific Reports, Frontiers in Microbiology, Bioanalysis, Frontiers in Bioscience, Phytomedicine, Current Metabolomics, etc., as well as resuming a peer-referee for National Natural Science Foundation of China, NHMRC in Australia and plus 20+ high-impact journals. **(Maximum: 350 words)**

Supplementary File 4: 会议回执返回至 chinmedomics2018@163.com

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