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Title: Discrimination of sepsis metabolic profiles revealed by LC/MS-MS based metabonomics approach

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Body: To identify metabolic biomarkers for differentiating sepsis from SIRS, and severity assessment, and outcome prediction. This study involved 35 patients diagnosed as sepsis, 15 patients with SIRS, and 15 normal controls. The contents of small metabolites and lipids in serum were measured by LC-MS/MS techniques and analyzed using multivariate statistical methods. The data from PCA revealed that normal and other patients with SIRS can be differentiated by metabolic profiles. Significant decrease ($P<0.05$) in the levels of Ne,Ne dimethyl-lysine, 27-Norcholestane hexol, dTDP-beta-L-rhodinose, Lactitol dihydrate, S-phenyl-D-cysteine, and PC(O-2:0/2:0) and increase ($P<0.05$) in the levels of Propenoyl carnitine, S-(3-Methylbutanoyl)-dihydrolipoamide-E, N-Nonanoyl glycine, and N-Nonanoyl glycine were observed in sepsis patients compared with the SIRS. The severe sepsis and septic shock were combined against sepsis, which represent sepsis severity, showed that lower levels in Propenoylcarnitine, Glycerylphosphorylethanolamine, Ne,Ne dimethyl-lysine, Galactosylhydroxylysine, 2-Phenylacetamide, D-Cysteine, and Phenylacetyl glycine ($P<0.05$). The profile of sepsis patients within 48h before death illustrated an obvious metabolic disorders state, S-(3-Methylbutanoyl)-dihydrolipoamide-E, 1,3-Dimethyl-uric acid, PG(22:2(13Z,16Z)/0:0), PG(14:1(9Z)/0:0), Epinephrine glucuronide, S-Succinyl-glutathione increased and Propenoyl-carnitine decreased ($P<0.05$). Computational network revealed that D-Cysteine played an important role during sepsis progress. From the view of metabolic kinetics process, Propenoyl-carnitine maybe a potential biomarker.