## Plasmonic Nanoshells Based Metabolite Detection for in-vitro Metabolic Diagnostics and Therapeutic Evaluation

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**Abstract :** In-vitro metabolic diagnosis relies on designed materials-based analytical platforms for detection of selected metabolites in biological samples, which has a key role in disease detection and therapeutic evaluation in clinics. However, the basic challenge deals with developing a simple approach for metabolic analysis in bio-samples with high sample complexity and low molecular abundance. In this work, we report a designer plasmonic nanoshells based platform for direct detection of small metabolites in clinical samples for in-vitro metabolic diagnostics. We first synthesized a series of plasmonic core-shell particles with tunable nanoshell structures. The optimized plasmonic nanoshells as new matrices allowed fast, multiplex, sensitive, and selective LDI MS (Laser desorption/ionization mass spectrometry) detection of small metabolites in 0.5 µL of bio-fluids without enrichment or purification. Furthermore, coupling with isotopic quantification of selected metabolites, we demonstrated the use of these plasmonic nanoshells for disease detection and therapeutic evaluation in clinics. For disease detection, we identified patients with postoperative brain infection through glucose quantitation and daily monitoring by cerebrospinal fluid (CSF) analysis. For therapeutic evaluation, we investigated drug distribution in blood and CSF systems and validated the function and permeability of blood-brain/CSF-barriers, during therapeutic treatment of patients with cerebral edema for pharmacokinetic study. Our work sheds light on the design of materials for high-performance metabolic analysis and precision diagnostics in real cases.

Keywords : plasmonic nanoparticles, metabolites, fingerprinting, mass spectrometry, in-vitro diagnostics

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