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High-throughput screening of protein-bound drugs and enzyme inhibitors using ambient mass spectrometry

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High-throughput screening (HTS) of protein-bound drugs and enzyme inhibitors is important for obtaining rapid understanding of drugs or enzyme inhibitors, which is significant in the developments of new drugs or mechanism studies in life science. Recently, ambient mass spectrometry has been applied for the rapid detection without sample pretreatment, which has potentials in real-time monitoring or high-throughput screening. In our group, several works on high-throughput screening of protein-bound drugs and enzyme inhibitors have been employed using ambient mass spectrometry. Firstly, we developed a rapid screening method for the detection of protein-bound small molecules using desorption electrospray ionization mass spectrometry (DESI-MS). The mechanism study on the interaction between DNA topoisomerase and inhibitors of camptothecin was carried out, and the relative binding strength was determined. Subsequently, the rapidly detection of 21 small molecule drugs has been successfully achieved within 1.75 minutes, enabling the high-throughput screening. In addition, a house-made platform combining with DESI has been constructed for examining the affinity between candidate ligands and anion-binding sites protein α1-acid glycoprotein, and the detection of 45 samples have been finished in 2.3 minutes. To further improve the high-throughput detection, a self-made protein microarray was fabricated combing with DESI-MS, which obtained the high-throughput examination of matrix metalloproteinase-9 interaction with 88 drug molecules. Furthermore, we used venturi easy ambient sonic-spray ionization mass spectrometry (V-EASI-MS) to monitor the binging affinity between drug and α1-acid glycoprotein in real time. By combining V-EASI-MS with liquid microfluidic technology, the high throughput screening of enzyme inhibitor drugs was further developed with a good stability, which achieved the detection frequency of 1.5s / sample. Therefore, the ambient mass spectrometry were effective in the high-throughput screening or detection of protein-bound drugs and enzyme inhibitors, which would show potentials in drug industry or clinical diagnosis.

Biography

Jin Ouyang received her Bachelor degree in Shaanxi Normal University, PR China and Ph.D. degree in Ghent University, Belgium. She is now working as a professor at Beijing Normal University, PR China. She is engaged in developing analytical methods based on mass spectrometry coupling to chromatography and electrophoresis, as well as applications of the methods to biological and pharmaceutical analysis. She received several Award such as the Chinese Female Analyst Award, China Association of Instrumental Analysis (CAIA) Award, and the State-level teaching famous teacher award. She published over 100 papers on peer-reviewed journals such as Anal. Chem., Adv. Funct. Mater., Chem. Commun., Nano lett., Small, etc.

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