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Direct and Comprehensive Analysis of Dyes based on Integrated Molecular and Structural Information via Laser Desorption Laser Postionization Mass Spectrometry

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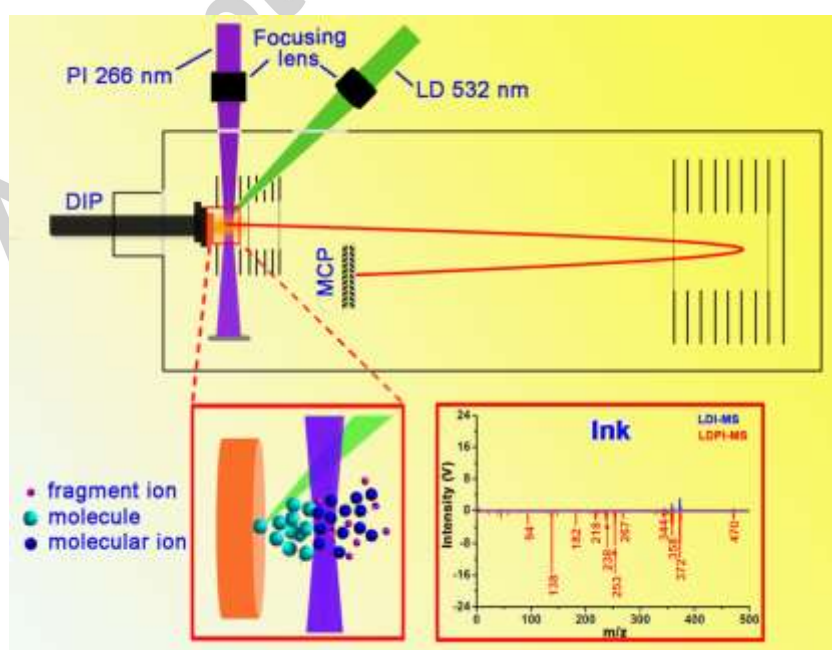
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Abstract

Laser desorption laser postionization time-of-flight mass spectrometry (LDPI-TOFMS) was employed for direct analysis and determination of typical basic dyes. It was also used for the analysis and comprehensive understanding of complex materials such as blue ballpoint pen inks. Simultaneous emergences of fragmental and molecular information largely simplify and facilitate unambiguous identification of dyes via variable energy of 266 nm postionization laser. More specifically, by optimizing postionization laser energy with the same energy of desorption laser, the structurally significant results show definite differences in the fragmentation patterns, which offer opportunities for discrimination of isomeric species with identical molecular weight. Moreover, relatively high spectra resolution can be acquired without the expense of sensitivity. In contrast to laser desorption/ionization mass spectrometry (LDI-MS), LDPI-MS simultaneously offers valuable molecular information about dyes in traces, solvents and additives about inks, thereby offering direct determination and comprehensive understanding of blue ballpoint inks and giving a high level of confidence to discriminate the complicated evidentiary samples. In addition, direct analysis of the inks not only allows the avoidance of the tedious sample preparation processes, significantly shortening the overall analysis time and improving throughput, but allows minimized sample consumption which is important for rare and precious samples.

Graphical abstract



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