

Electronic Supplementary Information (ESI)

Molecular imaging of small molecule drug in animal tissues using laser desorption postionization mass spectrometry

Jiixin Chen, Yongjun Hu*, Qiao Lu, Pengchao Wang, Huaqi Zhan

MOE Key laboratory of Laser Life Science & Institute of Laser Life Science,
College of Biophotonics, South China Normal University, Guangzhou 510631, P. R.
China.

* Corresponding author. Tel: +862119208713; fax: +862085216052

Email: yjhu@scnu.edu.cn

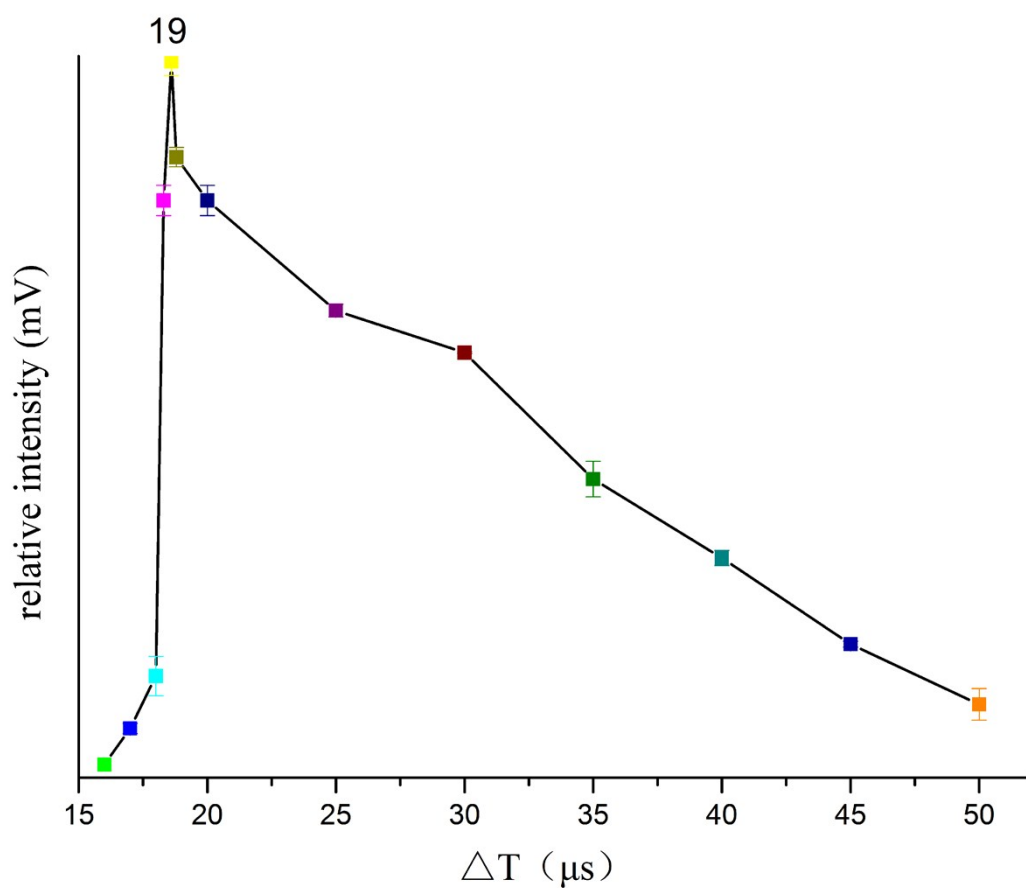


Fig. S1: The delay time (ΔT) distribution was plotted as the signal intensity versus the between the triggers of desorption and postionization lasers.

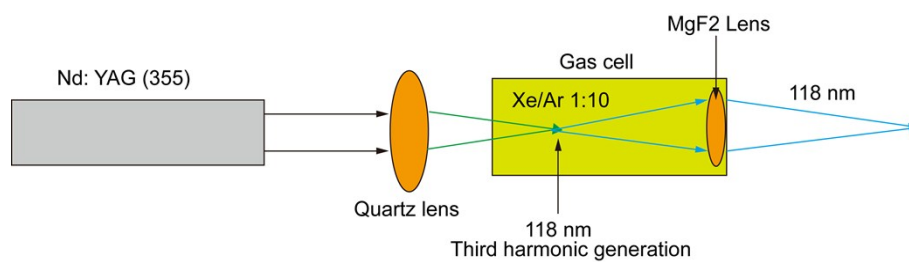


Fig. S2: The schematic diagram of VUV generation.

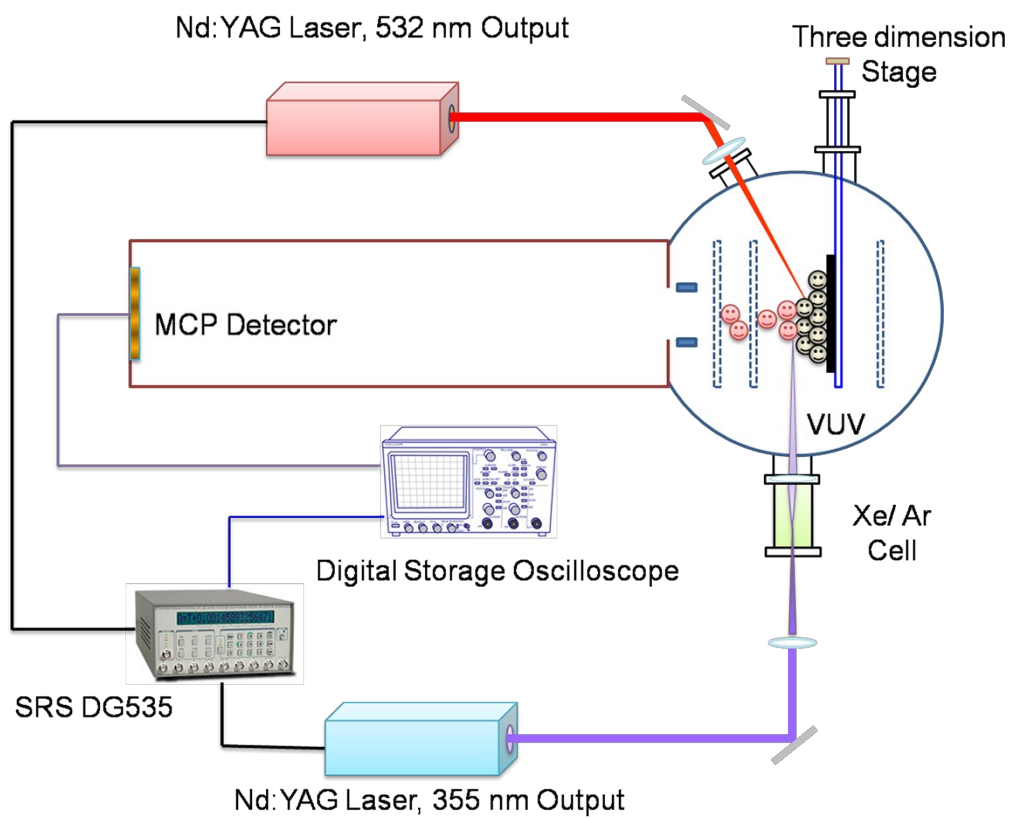


Fig. S3: The schematic diagram of the LDPI-MSI apparatus.

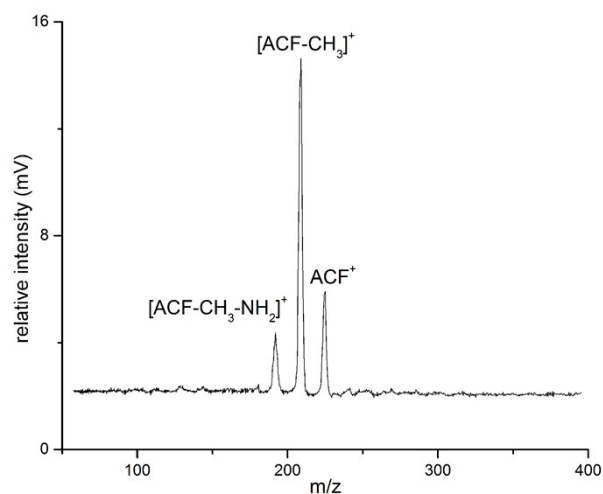


Fig. S4: The LDPI mass spectrum of pure acriflavine deposited directly on the corundum substrate, with obvious characteristic ions at m/z 193 ($[\text{ACF-CH}_3\text{-NH}_2]^+$), 209 ($[\text{ACF-CH}_3]^+$), and 224 (ACF^+).

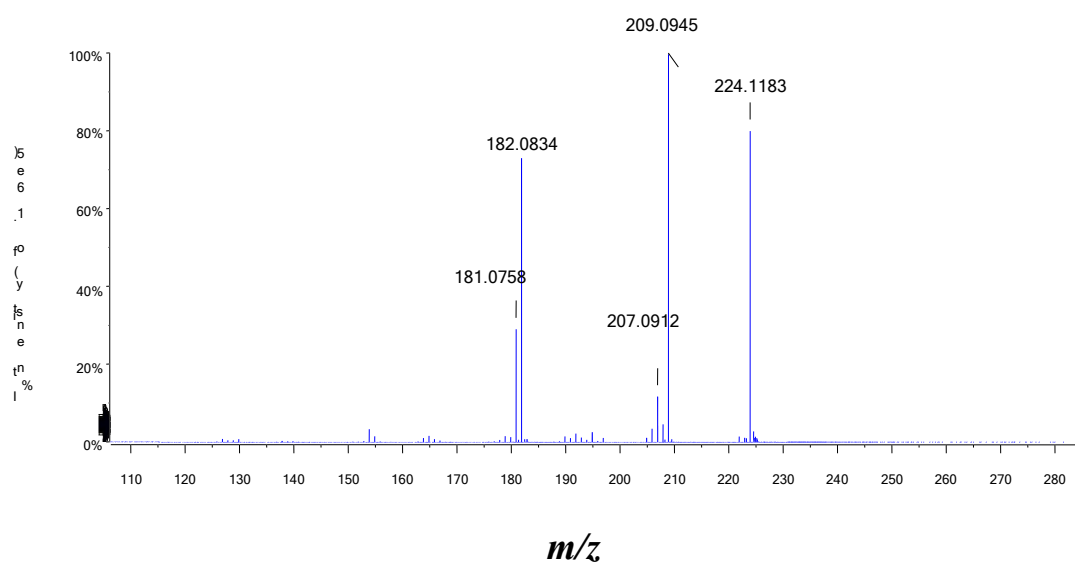


Fig. S5: DESI-MS/MS mass spectra of pure ACF with several similar fragment ions at m/z 209.0945 and 224.1183.

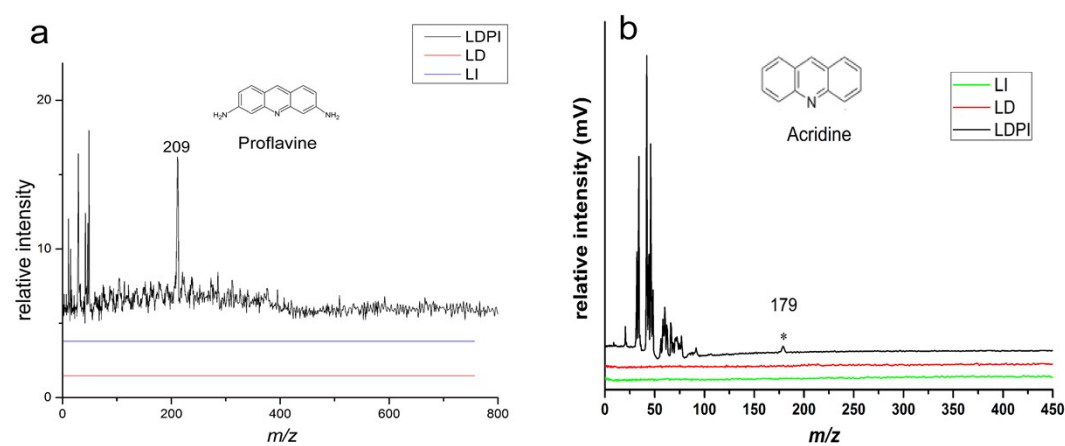


Fig. S6: LDPI mass spectra of **(a)** proflavine and **(b)** acridine-dosed mice kidney sections.

Supplemental Methods and materials

LC-MS/MS. The other half of each tissue sample was weighed before homogenization and extraction. To each tissue sample, a 0.1% formic acid in acetonitrile (5 mL) was added, and the resulting mixture was vortex-mixed for 5 min. Subsequently, the mixture was centrifuged at 3500 rpm for 15 min at 40°C, and the supernatant was decanted and transferred to a 50 mL conical tube. A further volume of 0.1% formic acid in acetonitrile (5 mL) was then added to extract the remaining residue. The supernatants were combined, and n-hexane (10 mL) was added. The mixture was vortexed for 30 s and centrifuged at 3500 rpm for 15 min at 40 °C. Aspirated 1 mL the lower layer mixed with 1mL 0.1% formic acid in wate and filtered through a 0.45 µm GHP syringe filter before analysis.

Quantitation was performed with a Thermo-Fisher Scientific TSQ quantum Ultra mass spectrometry in the positive ion mode. Analytes were separated by using a SHISEIDO (2.0 × 150 mm) column with a volumetric flow rate of 0.25 mL/min. The LC was connected directly into the mass spectrometer by using an ESI source.

The linearity of the calibration curve of LC-MS/MS was assessed by preparing kidney homogenates containing ACF at concentrations ranging from 5 to 500 ng/mL. The peak areas of ACF and concentrations were fit to straight by linear regression. The calibration curve and equation are

presented with their correlation coefficients

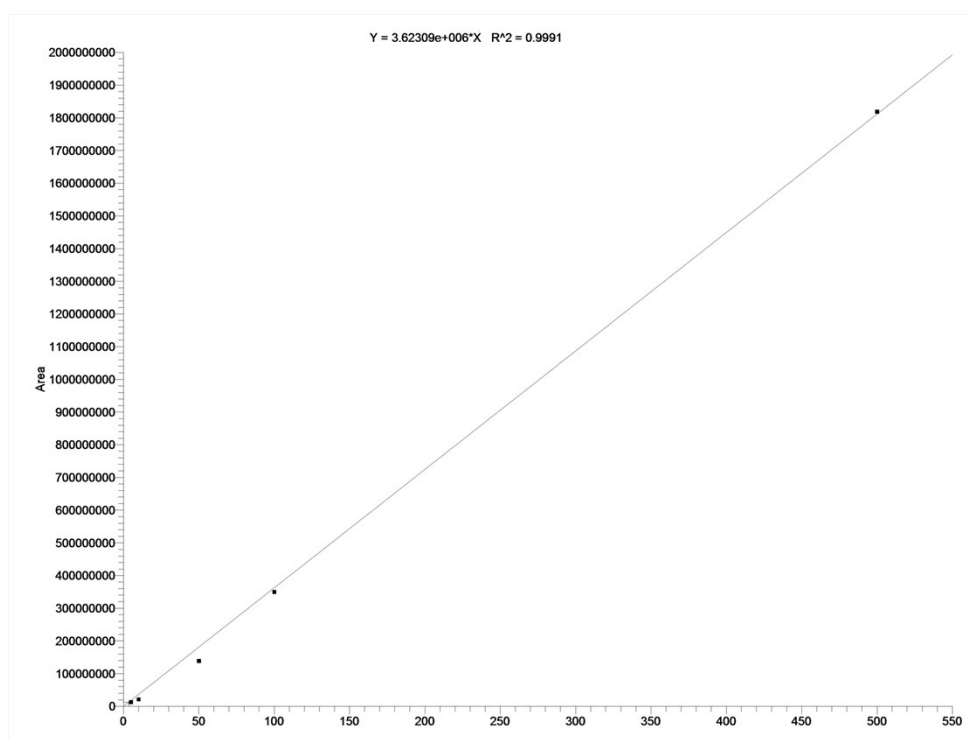


Fig. S7: The calibration curve of ACF with LC-MS/MS at concentrations ranging from 5 to 500 ng/mL.