Supporting Information

High Efficiency Tandem Mass Spectrometry Analysis Using Dual Linear Ion Traps

Linfan Li[1], Xiaoyu Zhou[1], James W. Hager[2], and Zheng Ouyang[1,3] *

1. Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN 47907
2. AB Sciex Pte. Ltd., 71 Four Valley Road, Concord, Ontario L4K 4V8, Canada
3. Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907

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* Corresponding Author

Prof. Zheng Ouyang
Weldon School of Biomedical Engineering
Purdue University
206 S. Martin Jischke Drive
West Lafayette, IN 47907-2032
Phone: +1 765 494-2214
Fax: +1 765 496-1459

I. Experimental

All chemicals were commercially available and used without purification. The amitriptyline-d6 was purchased from CDN isotopes (Pointe-Claire, Quebec, Canada). All other chemicals were obtained from Sigma-Aldrich (St. Louis, MO).

A bulk loaded sprayer, pulled from a boron silica glass capillary (0.85 mm i.d. and 1.5 mm o.d.), was used for nanoESI.

II. Instrumentation setups

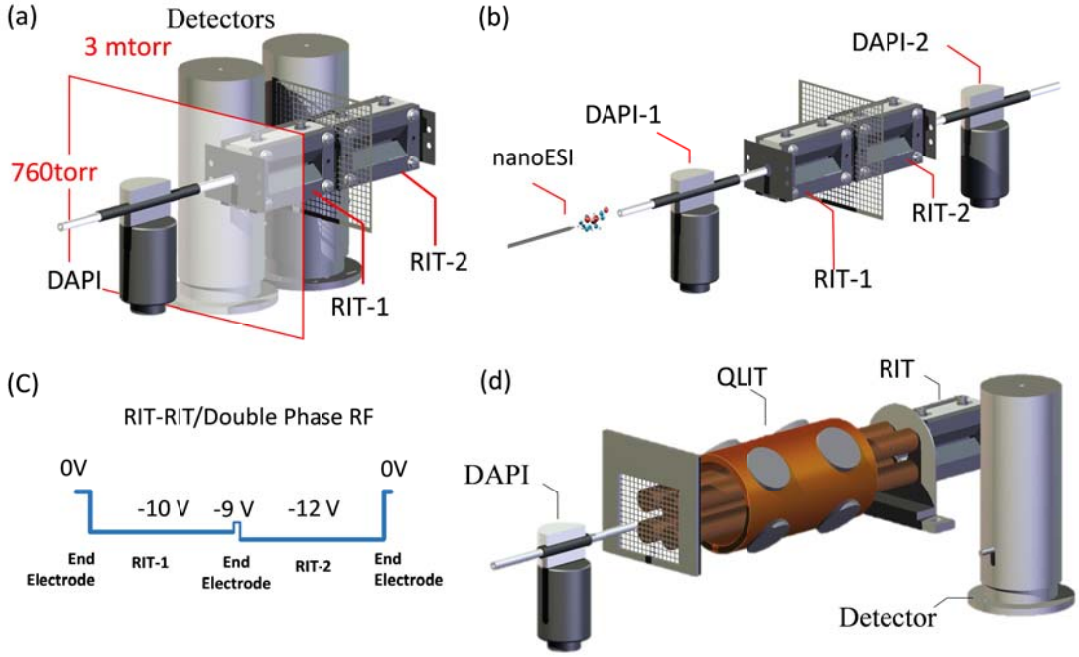

Figure S1. a) Instrument setup for testing the DAPI-RIT-RIT configurations. Two ion detector assemblies were used. The ions trapped in RIT-1 could also be monitored directly by an RF scan with radial ejection, for which the DC voltage on the common mesh end electrode was raised high (> 10 V) to prevent the axial ejection. The manifold pressure increased to about 500 mTorr with a 20 ms opening of the DAPI, which use a 500 µm i.d., 30 cm long capillary as the flow constraint. A delay of about 500 ms after DAPI opening was used to allow the manifold pressure to be pumped down to about 3 mtorr for MS or MS/MS analysis. The mesh electrode between two RITs was made from Corrosion-Resistant 304 Stainless Steel Woven Wire Cloth with an open area of 65% and wire thickness of 0.0075".

b) DAPI-2, with a 500 µm i.d., 35 cm long capillary as the flow constraint, was used to introduce air to increase the manifold pressure from 3 mtorr to 10 mtorr immediately before the mass-selective ion transfer.

c) The DC potential along the center axis during the mass-selective ion transfer in RIT-RIT driven by double phase RFs.

d) DAPI-QLIT-RIT setup with a single ion detector assembly.

The distances between the each end electrode to the adjacent RF electrodes are all 2 mm.

III. Characterization of the mass selective axial ejection of the ions by an RIT

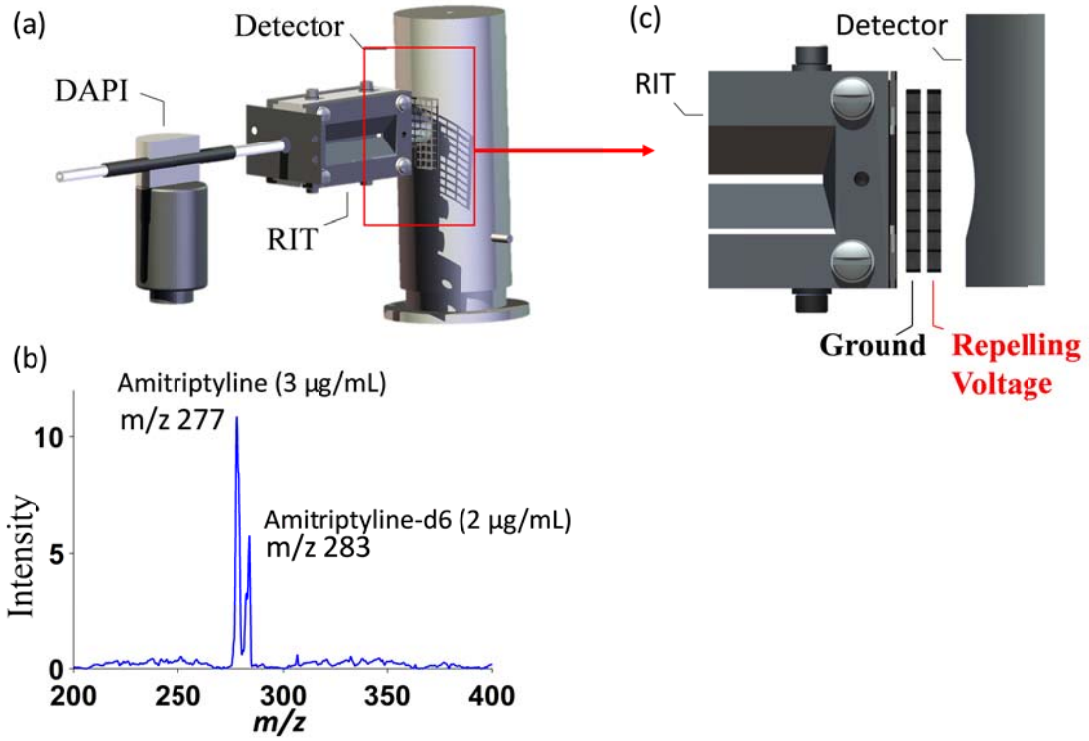

Figure S2. a) Instrument setup for detecting the axial ejection of the ions from RIT-1.

b) MS spectrum recorded for amitriptyline and amitriptyline-d6 (in methanol, ionized by nanoESI), single phase RF of 1.015 MHz applied on y electrode, dipolar AC applied between the x electrodes for resonance ejection at 165 KHz with 80 $mV_{p\text{-}p}$.

(c) An extra mesh electrode was inserted in front of the ion detector to apply a repelling potential. The kinetic energies of the ions axially ejected out of the RIT-1 needed to be high enough to overcome the barrier to reach the ion detector. By varying the repelling potential, the KE of the ions were profiled.

IV. Geometric impact on the electric field along the center axis of the LIT

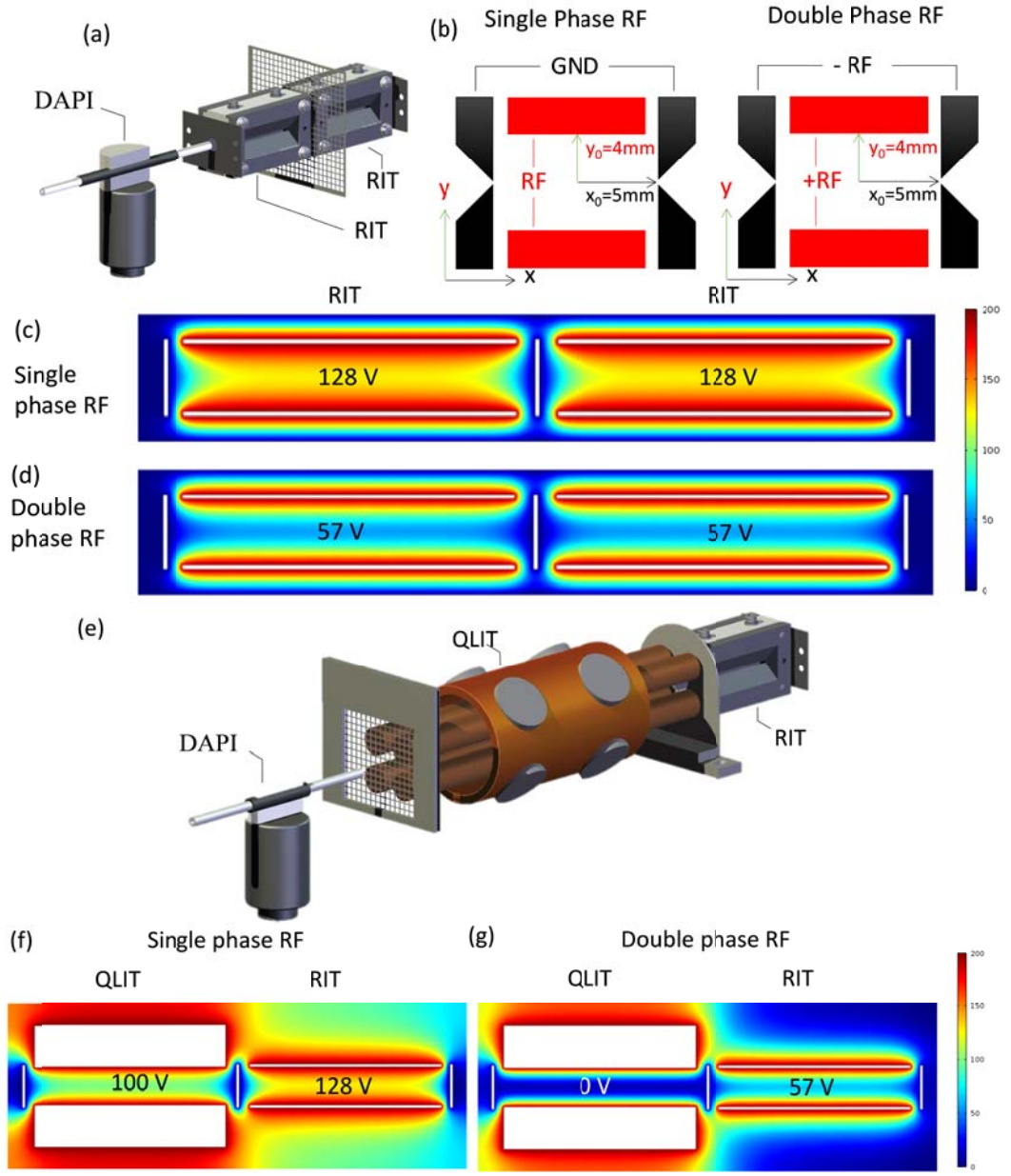

Figure S3. COMSOL (ver. 4.3a, COMSOL AB, Stockholm, Sweden) was used to solve the electric fields for the dual LIT configurations studied in this work. For a) RIT-RIT of b) stretched geometries, the potential along the center axis can oscillate at an amplitude as high as c) 128 V when a single phase RF of 200V is applied. d) With a balanced double phase RF applied between the x and y electrode pairs, the center potential is lower but could still be up to 57 V. For the e) QLIT with symmetric configuration, the center potential could still be high with the f) single phase RF but g) stays as 0 V when a balanced double phase RF is applied.

V. MS/MS analysis using DAPI-QLIT-RIT configuration

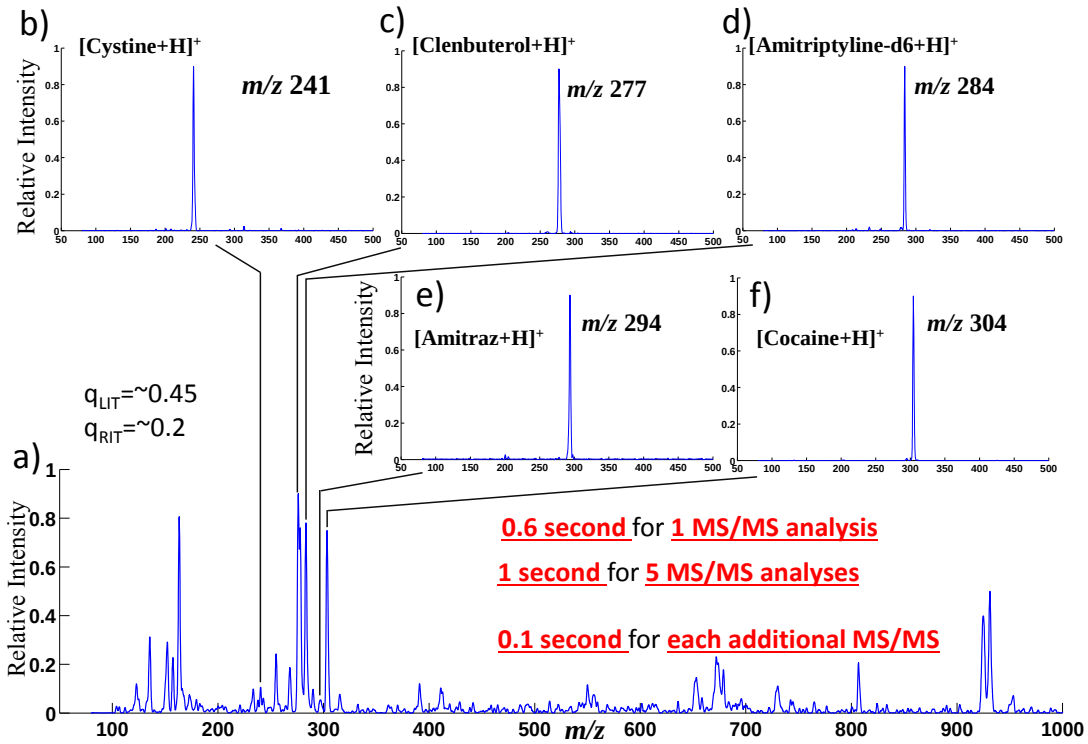

Figure S4. A mixture of clenbuterol (1 µg/mL), amitriptyline-d6 (1 µg/mL), amitraz (200 ng/mL), cysteine (500 ng/mL) and cocaine (500 ng/mL) in a methanol solution was ionized by nanoESI. The ions were introduced through DAPI and trapped in the QLIT. a) All the ions could be transferred to RIT without mass selection by lowering the potential on the common mesh electrode to -2.3 V. MS spectrum was recorded with a subsequent MS analysis using RIT with the radial ejection. b-c) While all the ions were trapped in the QLIT, the precursor ions in each narrow m/z range could be mass selectively transferred to RIT. When difference between the DC offsets of QLIT and RIT was smaller than 10 V, no significant fragmentation would occur. A subsequent MS analysis could generate MS spectra of the precursor ions as shown in b-f. MS/MS analysis could also be performed to each of these ions in RIT, with the results shown in Figure 2.

VI. Stability of the relative abundance for mass selective transfer from QLIT to RIT.

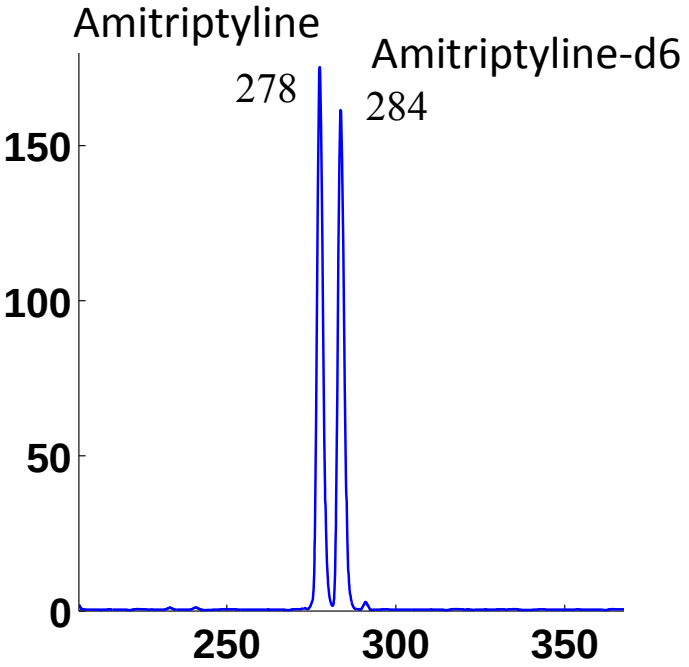

Figure S5. MS spectrum recorded for protonated amitriptyline m/z 278 and amitriptyline-d6 284, which were introduced to the QLIT at the same time but sequentially mass-selectively transferred to RIT with an interval of 100 ms. The measured intensities are used to plot the trends of the varying signals in Figure 4. Paper spray of methanol solution with amitriptyline and amitriptyline-d6 at 120 ng/mL, spray voltage of 4.3 kV. AC excitation of 80 mV 169 kHz, q = 0.45, for mass-selective transfer from QLIT. q = 0.2 for the trapping the ions in RIT.