SHIMADZU

WP 435

Prototype Development of a Digital Linear Ion Trap based Palmtop Mass Spectrometer

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1. Introduction

- Mass spectrometry is the gold standard for substance identification, particularly for trace sample detection. However, traditional mass spectrometers are still **bulky**, **power-consuming**, and **requiring highly skilled operators**, which makes them unsuitable for in-field scenarios such as emergency leak detection, drug abuse identification, and bedside monitoring.
- Currently, hand-held Raman, UV-VIS, GC, PID, FID and ion mobility spectrometers have been widely used in these scenarios discussed above. However, current solutions cannot have outstanding qualitative and quantitative capability simultaneously (**Fig.1**).
- To address this issue, we have developed an ultra-compact Palmtop MS (PMS) which can be held in hands and can also be carried by a UAV or robot. This prototype has the potential to expand the application areas for MS instruments, similar to how mobile phones brought more possibilities in the PC era.

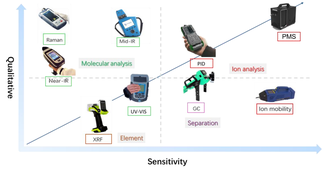

Fig. 1 Current palmtop analysis instruments solutions comparison

2. Methods

- The PMS is based on Shimadzu's digital linear ion trap technology with a field radius of only 3 mm. This allows for low RF amplitude and low-power consumption. We chose a 10.6 eV Kr VUV lamp as the ionization source to meet demands from environmental applications. The sample molecules were transmitted into the ion trap through a PDMS membrane interface. Upon entering the ion trap, the neutral molecules were ionized by the VUV lamp mounted on the opposite side of the trap. The vacuum was maintained at the level of 10E-3 Pa with a combination of a Non-Evaporable Getter (NEG) pump and an ion pump, after being exhausted by a TMP (**Fig.2**).
- A partition wall with an aperture was used to divide mass analyzer and pump group into two chambers to create a suitable pressure for ion trap (*US20230352291A1*).

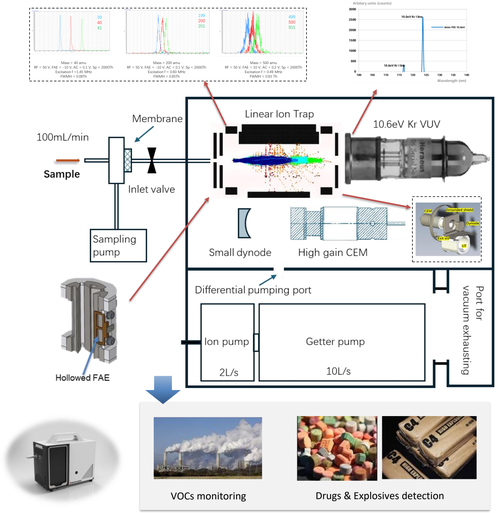

Fig. 2 PMS solution schematic

3. Results

- The core characteristics of the MS part have been validated in the current prototype. The mass range can be from 40 Th to 500 Th and the unit resolution (FWMH<0.8 Th) is achieved throughout the mass range. The CV in 40 minutes of continuous sampling is below 5% (**Fig.3**). The limit of detection (LOD) can be around 10 ppb for toluene and 10 ng for drugs (e.g., MDMA).
- Currently, the PMS weights ~6 Kg, and has a working power of around 30 W (2 hours lifetime with 60 W·h Li-battery), the dimension of the prototype is 270(L)*190(H)*135(W) mm, which can be lifted with one hand or held with two hands.

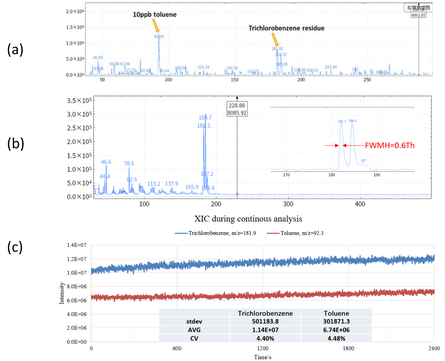

Fig. 3 MS performance test experiment data. (a) LOD, signal of 10 ppb toluene (b) Resolution, signal of 1 ppm trichlorobenzene. (c) stability, signal of 1 ppm VOCs 40-mins continuous sampling.

- The sampling port is designed to be modularized (**Fig.4)** in order to be used independently or coupled with either GC or a thermal desorption source which give rise to extreme complex VOCs mixture analysis and solid/liquid sample analysis, respectively.

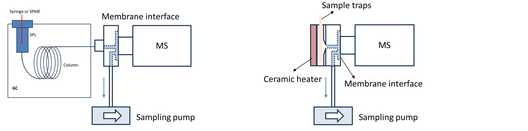

Fig. 4 Different sampling port. GC interface (left), thermal desorption port (right).

- Now, we have successfully identified more than **30 VOC substances** among the TO-15*, **9 drugs** and **6 CWA simulants** (chemical weapon agents simulants). For the drugs, the majority of which exhibits significant dissociation with the PI source. And large molecular substance, such as fentanyl, response is still not high enough which may be caused by the condensation during transmission. In the case of CWA simulants, a very good response is obtained with most substances yielding precursor ion signal (**Table.1** and **Fig.5**).

*TO-15: a mixture standard of 65 VOCs

	MW	SNR	Precursor ion
Chemical warfare agent (CWA) simulants			
DMMP	124.1	44ng (SNR=10)	Yes
TMP	140.1	210ng (SNR=12)	Yes
TEP	182.1	213ng (SNR=10)	Yes
TPP	224.2	83ng (SNR=25)	Yes
TiPP	224.2	59ng (SNR=10)	Yes
Profenofos	373.6	25ng (SNR=3)	Yes
Drugs			
MDA	179	20ng (SNR=60)	No
Amphetamine	135	10ng (SNR=10)	Yes
Safrole	162	100ng(SNR=50)	No
Methamphetamine	149	100ng (SNR=40)	Yes
MDMA	193	10ng (SNR=20)	Yes
Pseudoephedrine (+)	165	100ng (SNR=130)	No
Ephedrine (-)	165	25ng (SNR=160)	No
Fentanyl	336.5	28μg (SNR=50)	No
AB-CHIMINACA (cannabis)	356.5	16μg (SNR=80)	No

Table.1 Experiment results of typical drugs and CWA simulants in the PMS prototype

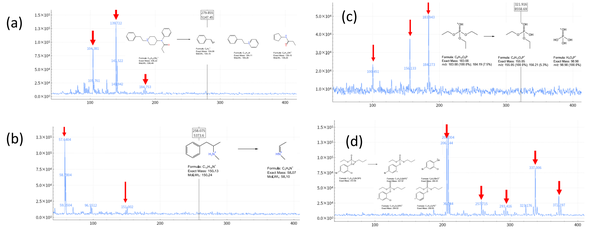

Fig.5 MS spectrum of detected drugs and CWAs simulants. (a) 28 ug fentanyl, (b) 100 ng Methamphetamine, (c)213 ng TEP, (d) 250 ng Profenofos.

4. Conclusion

- A prototype of the palmtop MS has been developed. The total weight is ~6 Kg with dimension of 270(L)*190(H)*135(W) mm and 2 hours battery life. The mass range is 40 Th ~ 500 Th within which the **unit resolution** can be achieved.
- The prototype has been used in VOCs detection, drugs and CWA simulants identification. The next step will involve exploring more scenarios, particularly for in-field application cases, for PMS.
- There is still considerable scope for optimization in terms of sensitivity and the number of detectable substances. Efforts will also be made to reduce the size, weight and power consumption of PMS, thereby enhancing its suitability for on-site users.