

Fundamental Principles and Performance for a Low Vacuum Mass Spectrometer

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1. Overview

This research is intended to further enhance the robustness and reduce the size and cost of portable mass spectrometer by getting rid of turbo pump without sacrificing much of performance.

2. Introduction

A low vacuum mass spectrometer (LVMS) was developed to be operated at a pressure of ~ 10 Pa without using turbo pump. FWHM ≤ 1 Th can be achieved for mass range of 18 – 400 Th. Such miniature prototype was developed for VOCs detection with membrane inlet or coupling with microGC for enhanced qualitative gas analysis.

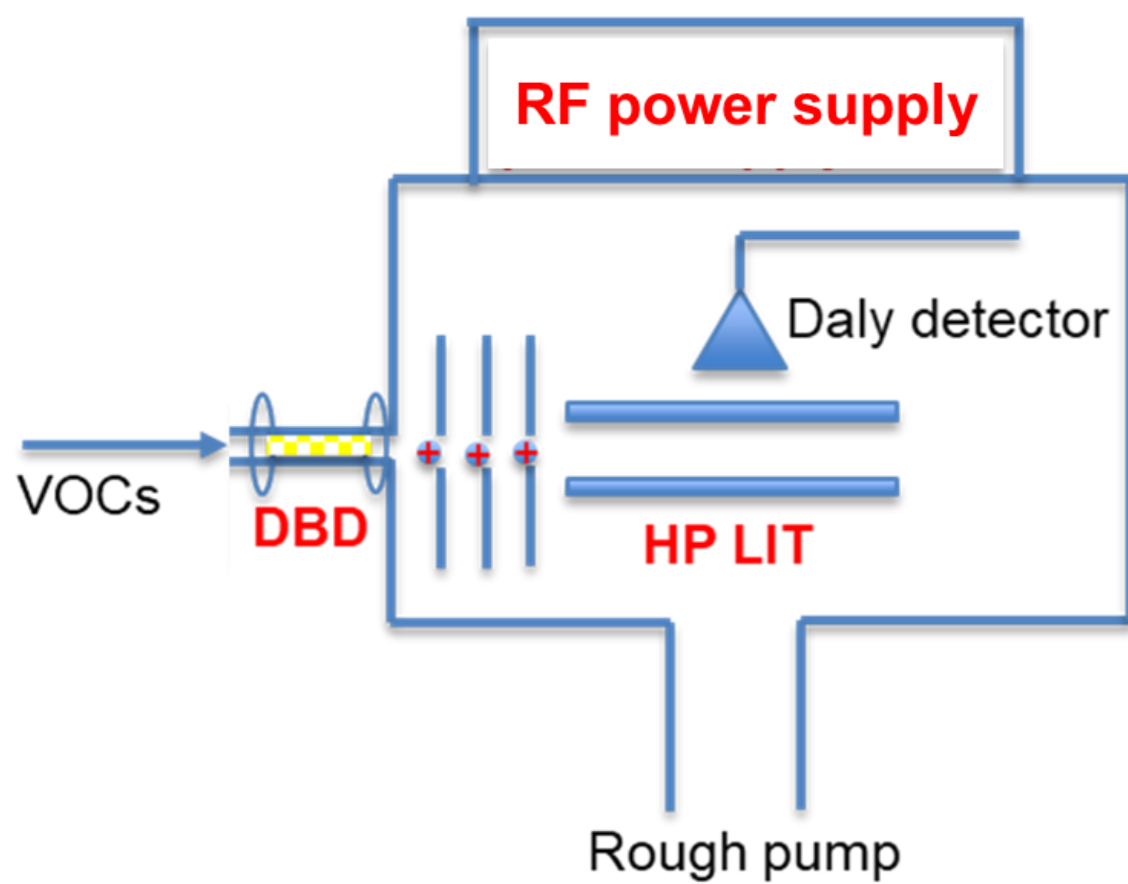


Figure 1 Configuration of LVMS.

3. Methods

To operate at intermediate pressure (~ 10 Pa), a high pumping speed rough pump is used to reach a low ultimate pressure. VOCs are ionized by a low pressure dielectric barrier discharge (LP-DBD) source. A linear ion trap (LIT) is used as mass analyzer. RF frequency of 6 MHz is used to reach good resolution. FWHM ≤ 1 Th can be obtained both in simulation and experiments. To operate at high pressure, a Daly detector is used of which the maximum operating pressure is ~ 4 Pa.

4. Results

4-1. LIT simulation

Simulation conditions	
Software	AXSIM2016
Collision model	Combined Langevin and hard-sphere
Pressure	2-10 Pa
Ion trap	Linear ion trap (LIT)
Driving RF frequency	6 MHz
Simulated ions	Reserpine 609 Th, 610 Th and 611 Th

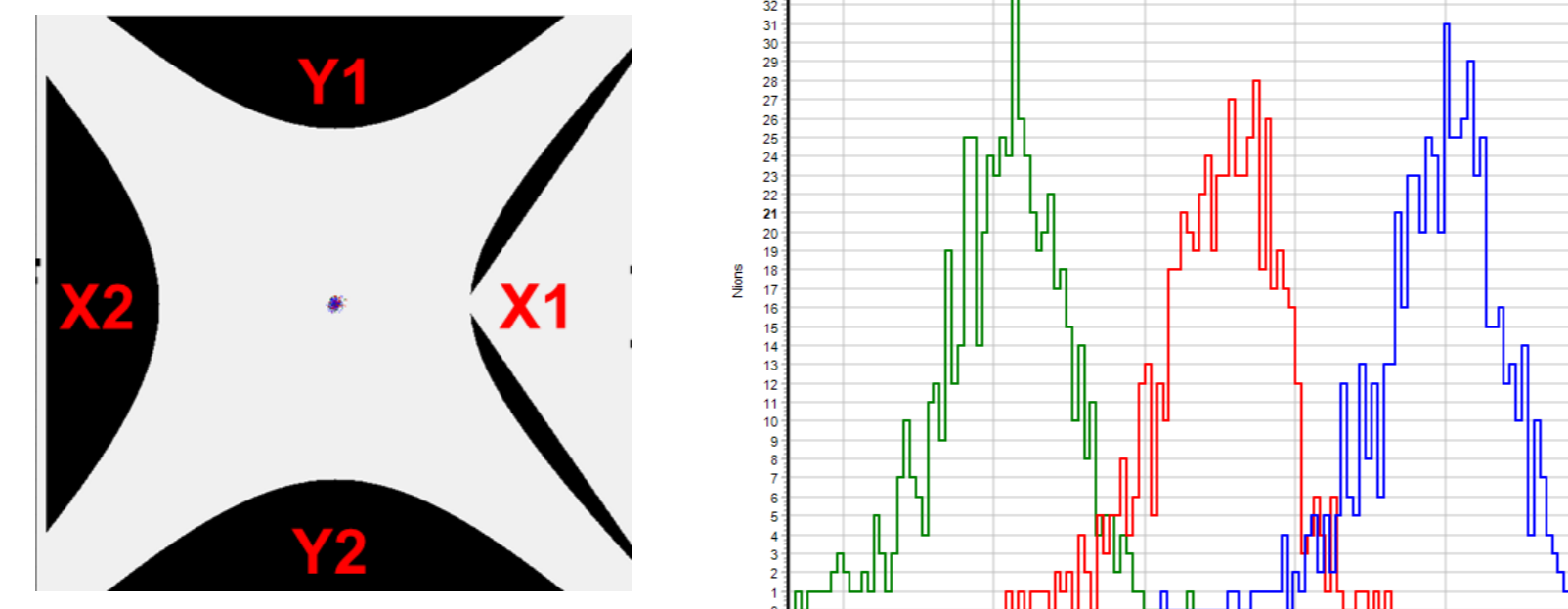


Figure 2 Simulation of LIT at 2 Pa. FWHM = 0.6 Th and > 40% of ejection rate can be achieved by 6 MHz RF frequency.

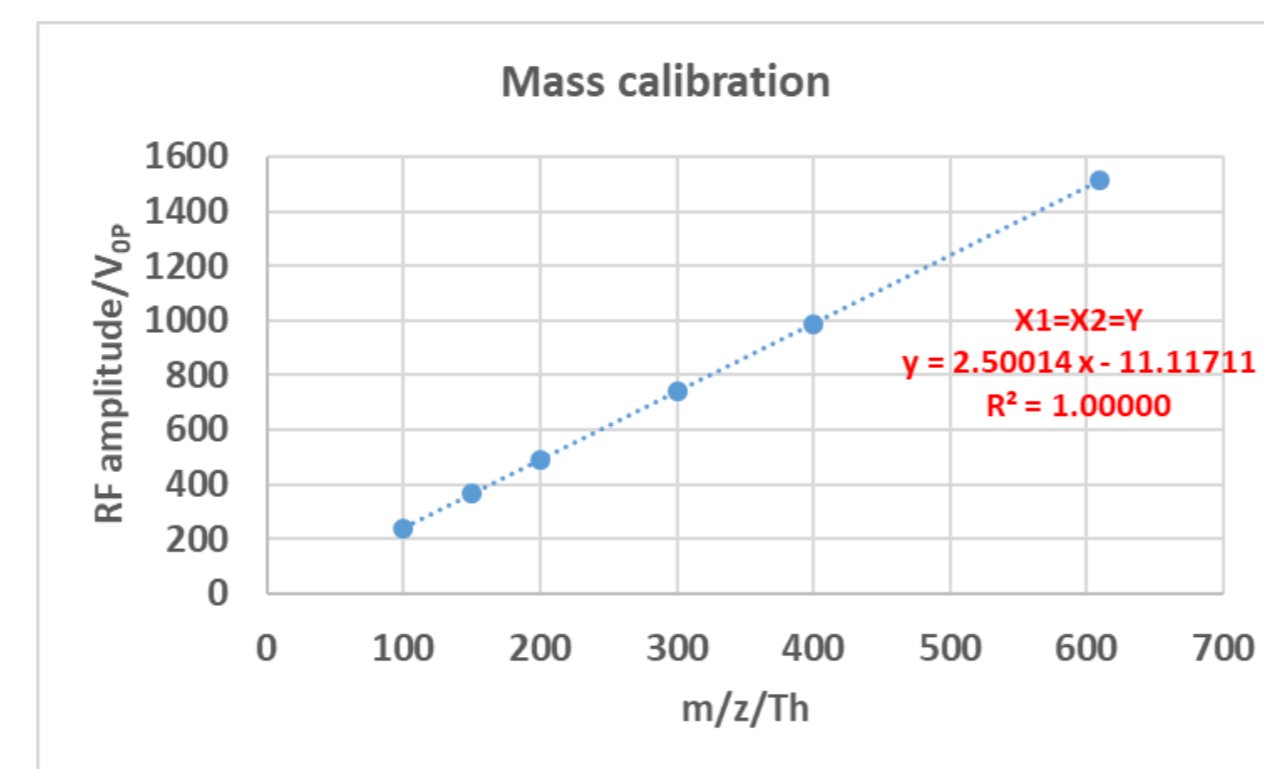


Figure 3 shows the calibration line of m/z VS RF 0-peak amplitude in simulation. Very good linearity can be obtained. The calibrated m/z deviates ≤ ± 0.3 Th from real value.

4-2. LP-DBD ionization source

The workable intermediate pressure ion source is a big challenge. EI filament will burn out. On the other side, this pressure is too low for DC GD which is impossible to produce stable discharge. The pressure independent photoionization may be a good choice. But commercial photoionization lamps with enough irradiance only have maximum output photon energy of 10.76 eV, which can't cover all of ionization potentials of VOCs.

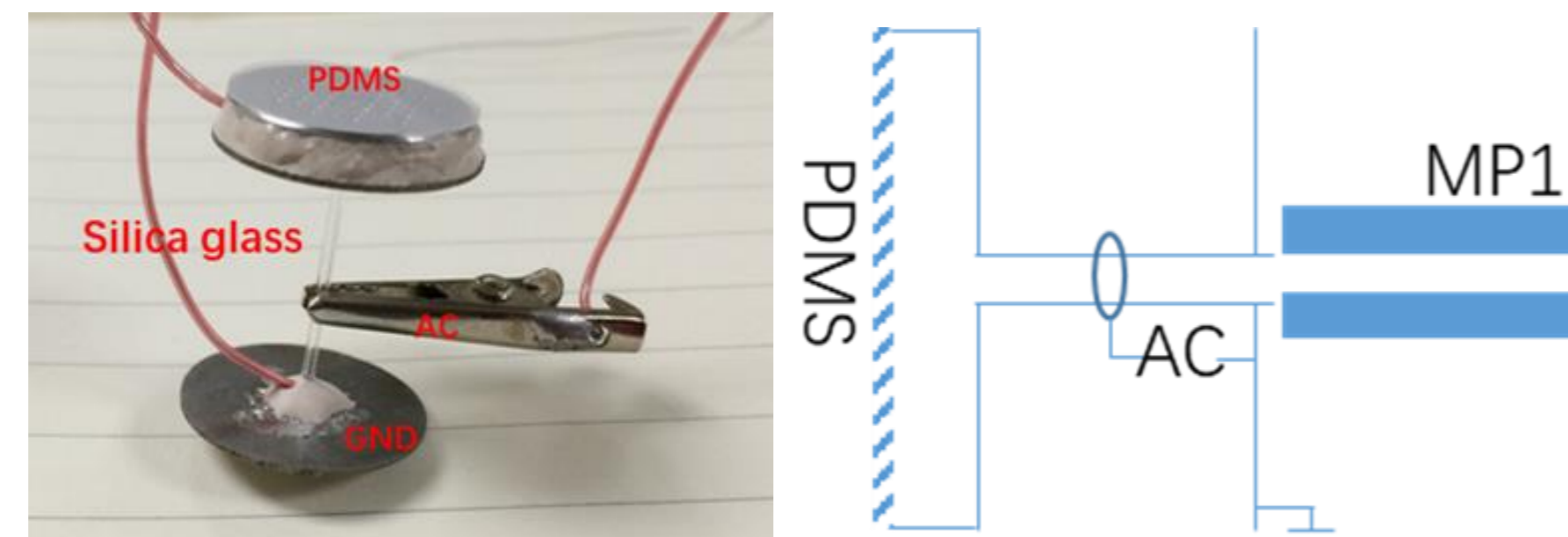


Figure 4 Structure of DBD source on Shimadzu LCMS8040®. The PDMS membrane thickness is 50 μm.

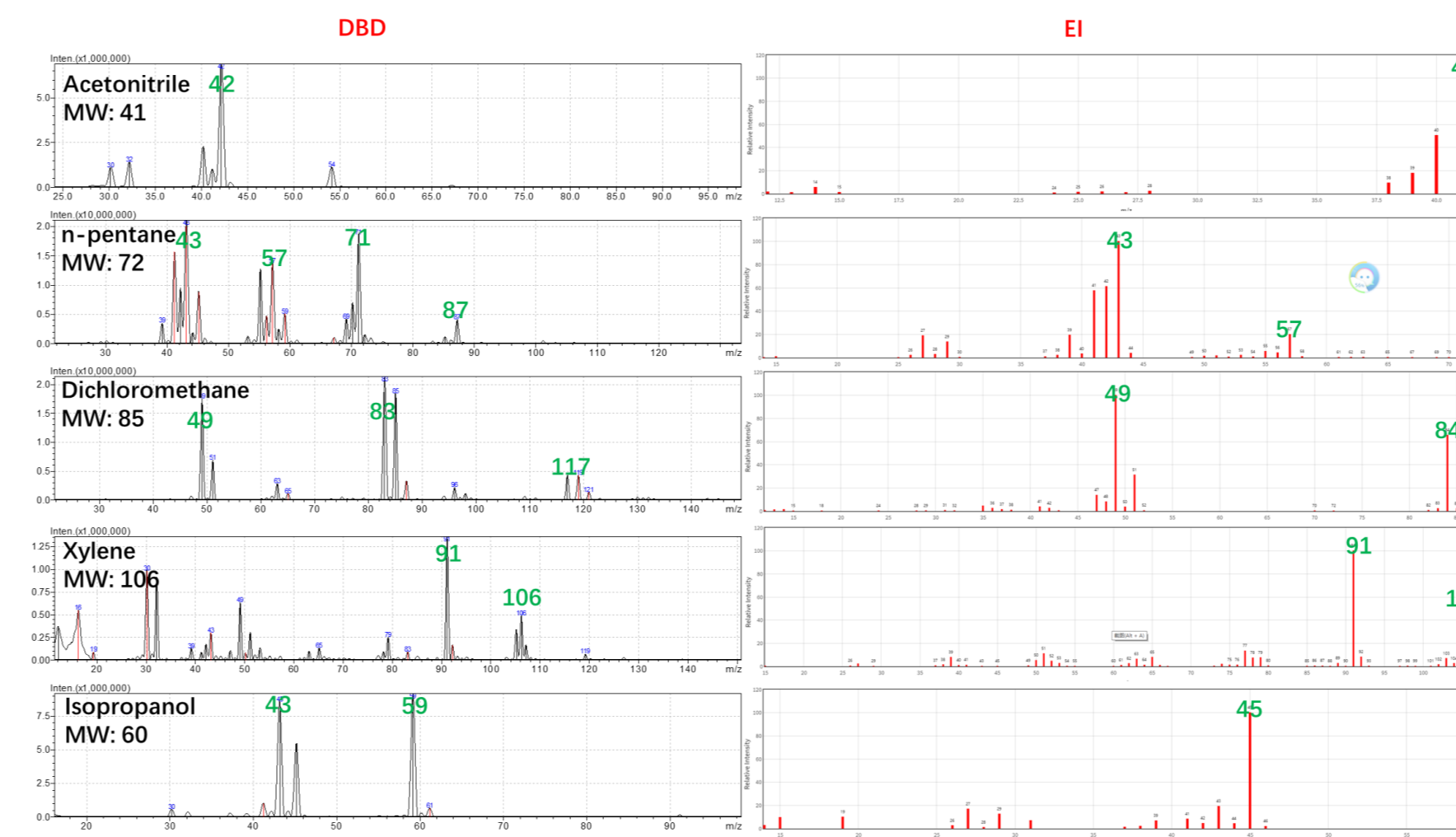
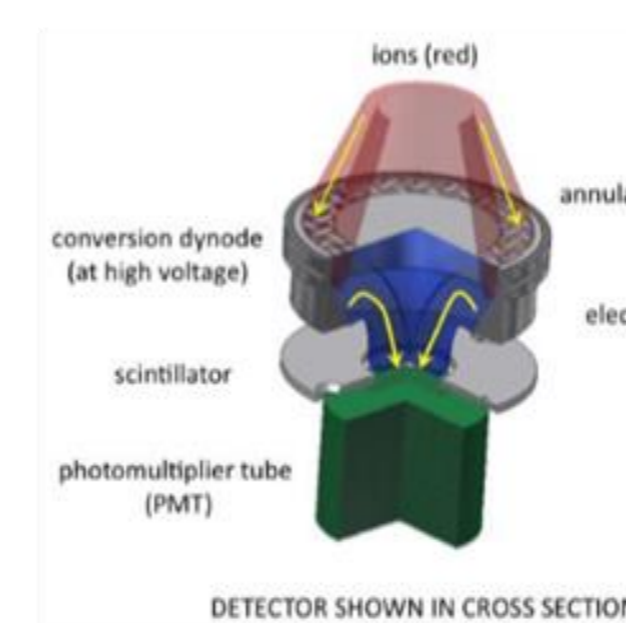


Figure 5 Representative mass spectra of acetonitrile, n-pentane, dichloromethane, xylene, and isopropanol by DBD ionization and standard EI from NIST.

4-3. Detector selection

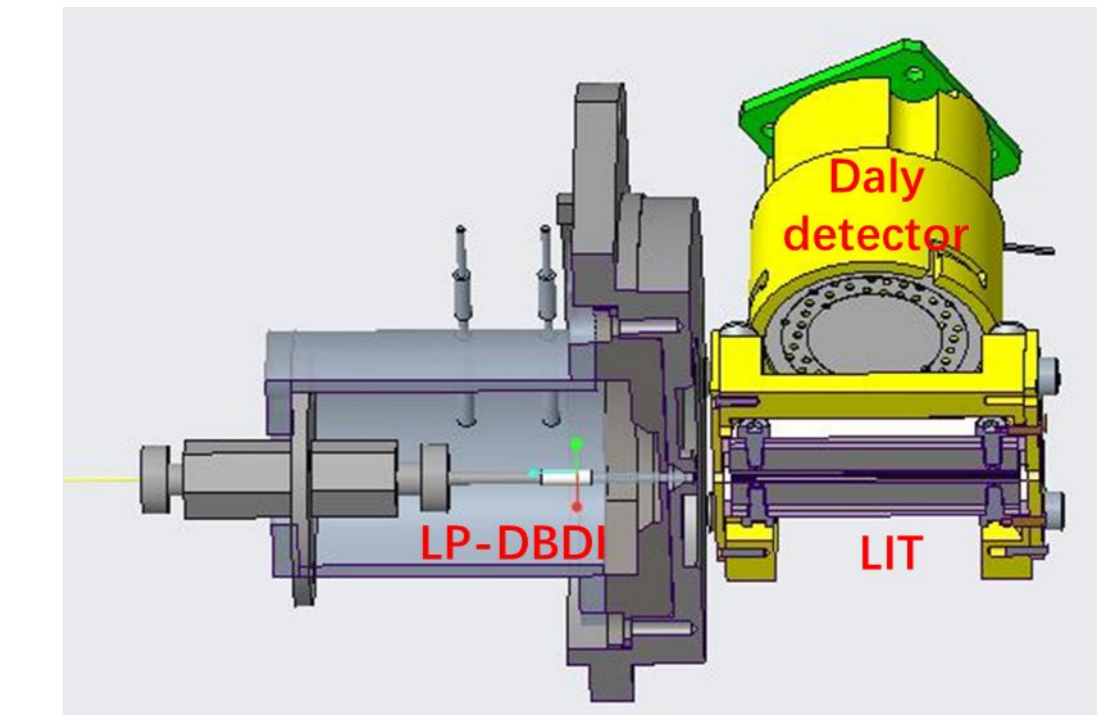
Figure 6 Cross section; physical and electrical characteristics of Daly detector developed by Photonis.



Physical Characteristics	
Annular Input Dimensions	22 mm OD 16 mm ID
Input Grid	60% Transmission (16 mm ID is occluded)
Operating Pressure (Maximum)	30 mTorr
Operating Temperature Range	-50° to +40° C
Electrical Characteristics	
Dynode Voltage	1500 – 5000 V
PMT Voltage	-600 V (-1100 V Max)
PMT Current	< 360 μA
Signal Response Time	< 100 ns
Detector Gain	> 5E5
Detector Dark Current	< 5 nA

The gain is very stable during 30 mins of test and shows independence of background pressure (~ 3200 of gain at 0.08 – 2.3 Pa). The gain is increasing with conversion dynode voltage because at first, more electrons are generated and at second, the higher voltage gives electrons more energy and more energetic electrons produces more photons from the scintillator. The gain is even more sensitive to the PMT voltage since it is most important part from which gain is obtained. An increase of 200 V PMT voltage will cause 10 times increase of gain. Short-term evaluation shows the detector has high and stable gain at 2.3 Pa of air.

4-4. LVMS prototype development



The prototype is based on one stage vacuum system. Only a rough pump is used. RFPS is mounted at a position to reach the minimum connection distance between output and LIT electrodes. A makeup gas is supplied from any gas type to reach desired pressure. LP-DBDI is used as ion source which can be replaced by photoionization easily without any other changes.

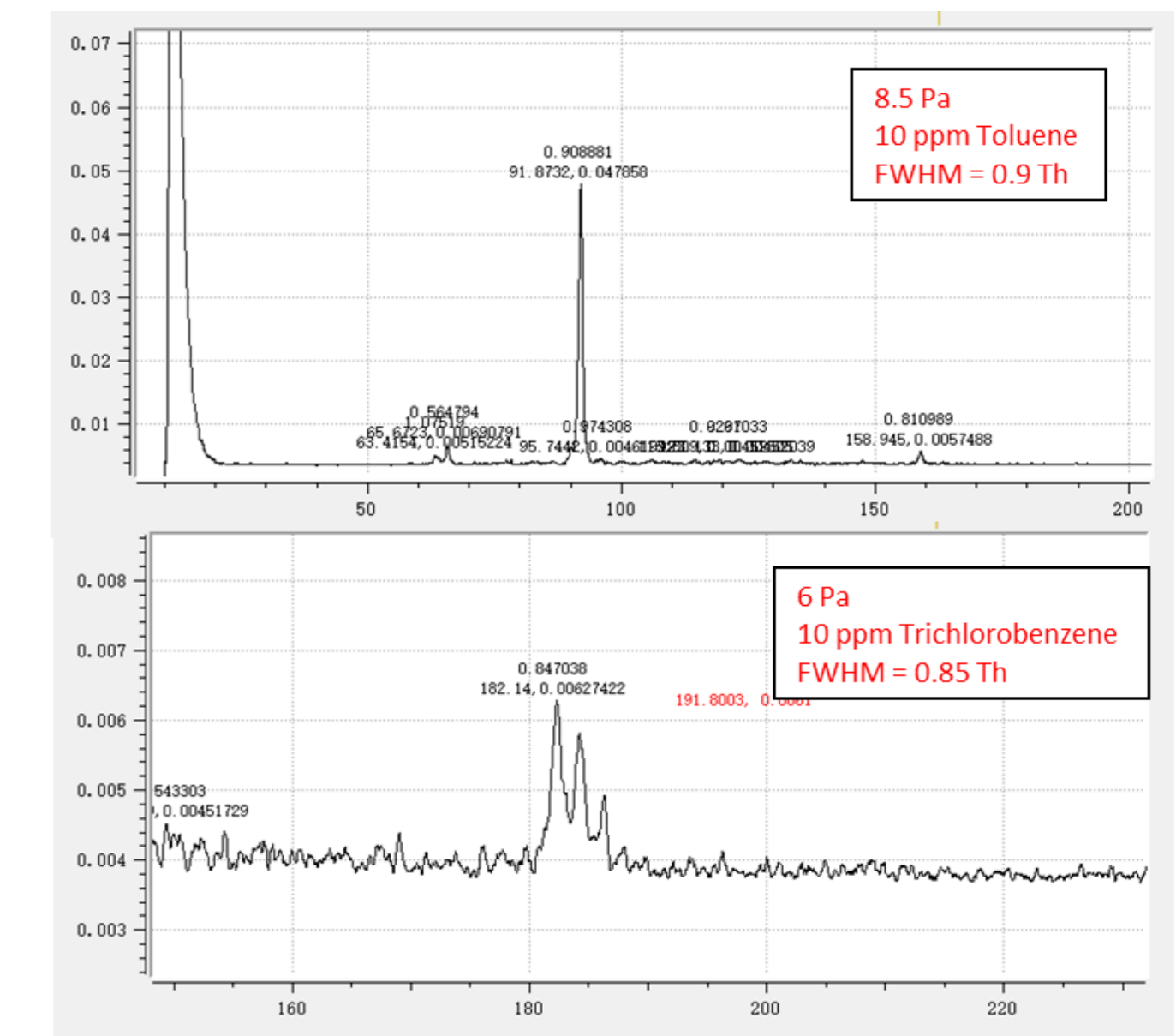


Figure 7 FWHM ≤ 1 Th is reached for toluene at 8.5 Pa and trichlorobenzene at 6 Pa.

5. Conclusions

A LVMS prototype was setup by using only a rough pump. FWHM ≤ 1 Th can be reached at ~ 10 Pa for full mass range of 20 – 400 Th. The prototype can be used independently with membrane inlet or coupled with micro-GC for enhanced performance.