Differential Mobility Ion Pre-filter for Field - Deployable Atmospheric Pressure Ionization Mass Spectrometers

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Objective

Detection of target chemicals in complex environments such as public spaces (for example, administrative buildings, shopping malls and subway systems) is problematic when utilizing atmospheric pressure ionization (API) mass spectrometry (MS). This is mainly due to complex gas phase processes, which lead to the formation of a large number of ionic species and their cross interactions in the ionization region. Therefore the presence of numerous interferences in such harsh environments increases false alarm rates, frequently to unacceptably high levels.

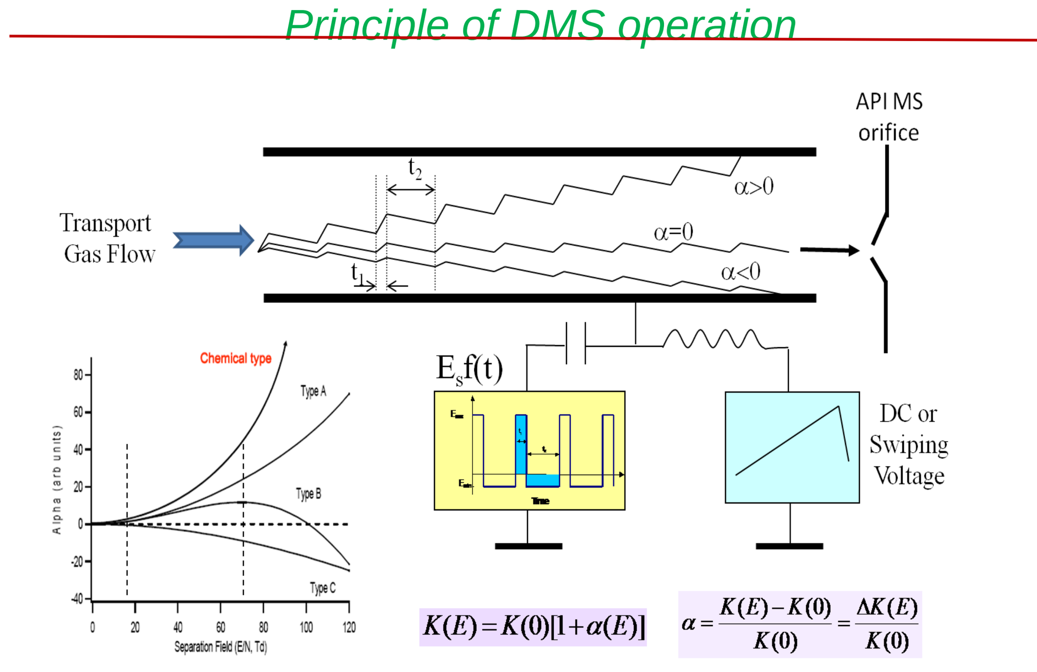
An effective method to avoid these challenges is to combine MS with other fast-operating separation methods. This approach enhances the detection accuracy of the system as a result of: (a) selection of targeted ion species before introduction in the MS and (b) providing additional orthogonal chemical information for targeted species.

In this poster, we will present design concepts and expected benefits of using planar DMS as a pre-filter for miniature MS. The proposed designs are intended to operate with various types of fieldable API-MS systems equipped with capillary inlet sample introduction. Progress towards development of such a system will be presented.

DMS interface operation principle and output

Planar Differential Mobility Spectrometry (DMS) is a rapid ion separation method, which can operate as a standalone spectrometer and can provide mobility spectra for positive and negative ion species. DMS can also be employed as a continuous ion filter for targeted ion species. In the latter case, DMS can be tuned for filtration of selected ions of interest and for effective removal of other undesirable interfering ion species prior to analysis by MS.

Principle of DMS operation



Mathematical description of method

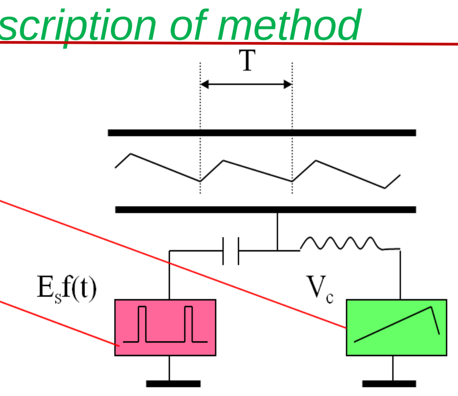
$$K[E(t)]=K(0)[1+\alpha(E)]$$

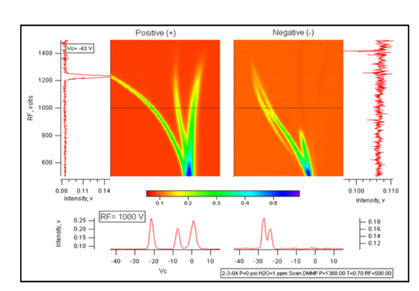
$$E(t)=E_s(t)+V_c/d=E_s f(t)+V_c/d$$

$$\vec{\vartheta}(t)=K(E)\times\vec{E}(t)$$

$$\upsilon=<\upsilon(t)>=\frac{1}{T}\int K(E)E(t)dt=0$$

$$V_c=\frac{<\alpha E_s f(t)>d}{1+<\alpha>+<\frac{d\alpha}{dE}E_s f(t)>}$$

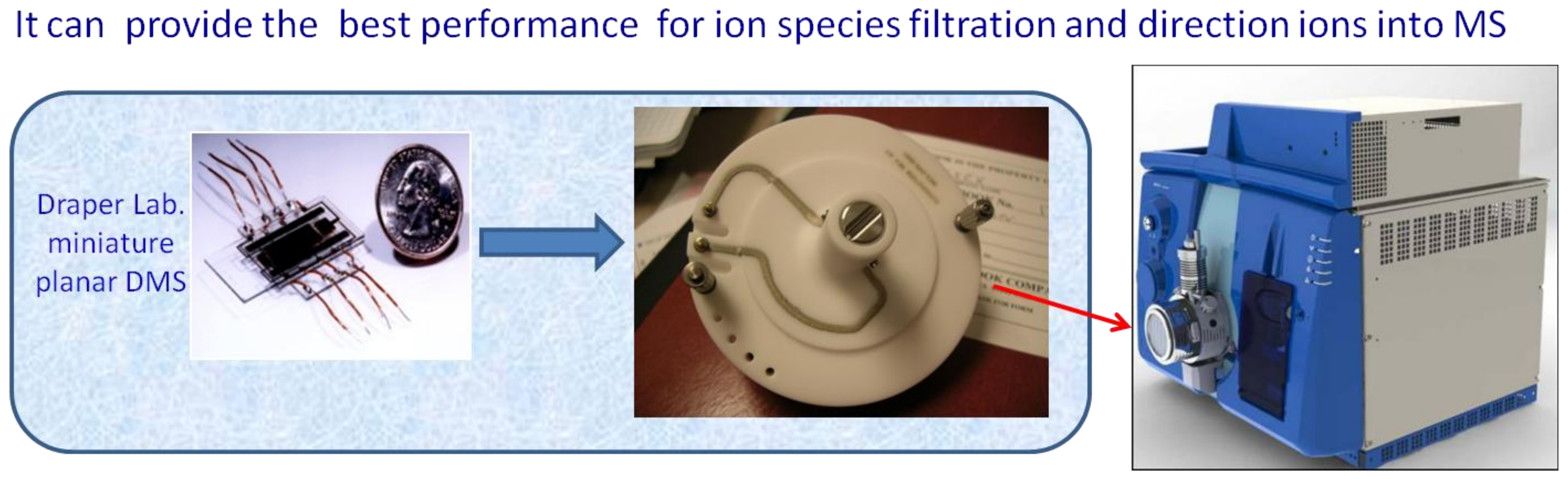




AB Sciex recently released SelexION^{TM}

The SelexION™; combining DMS and MS (Triple Quad5500^{TM} or QTRAP 5500) provides proven improvements in scan speed, tuning stability, separation power (through the use of chemical modifiers), reliability and robustness, and chemical noise reduction.

Simple and robust planar DMS design is ideal for building the tunable interface for API MS.
It can provide the best performance for ion species filtration and direction ions into MS

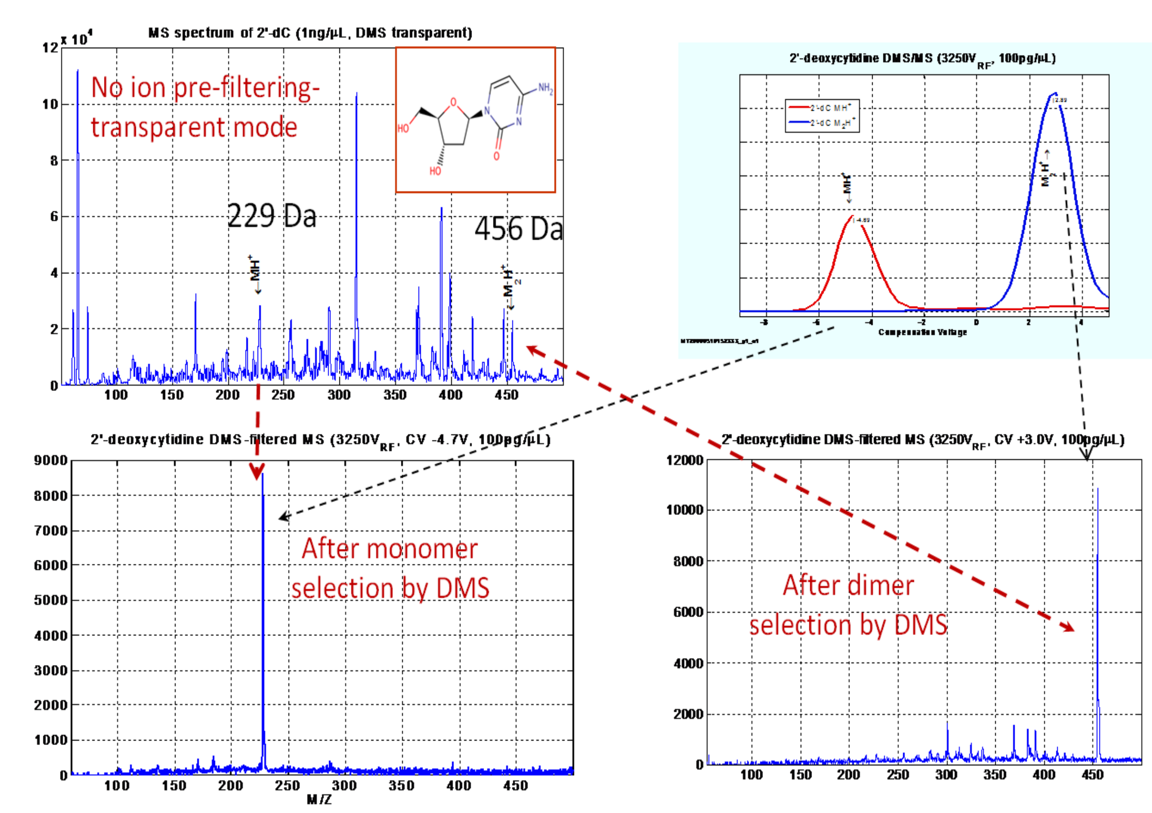


Advantages for using Planar Design DMS Interface

#1 Provides a transparent mode of operation.

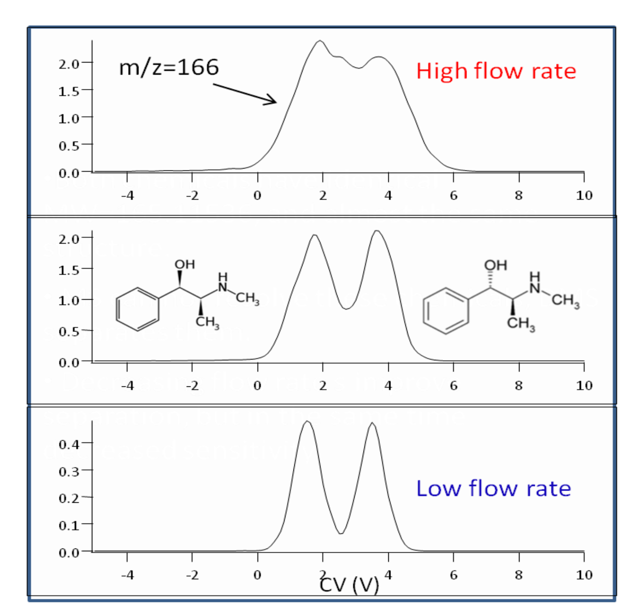
#2 In regime of filtration substantially decreases chemical noise which is especially valuable for small molecule samples.

Example: **Detection Radiation Biomarker in Urine samples(2'-Deoxycytidine) MW 228, 100 pg/μL**



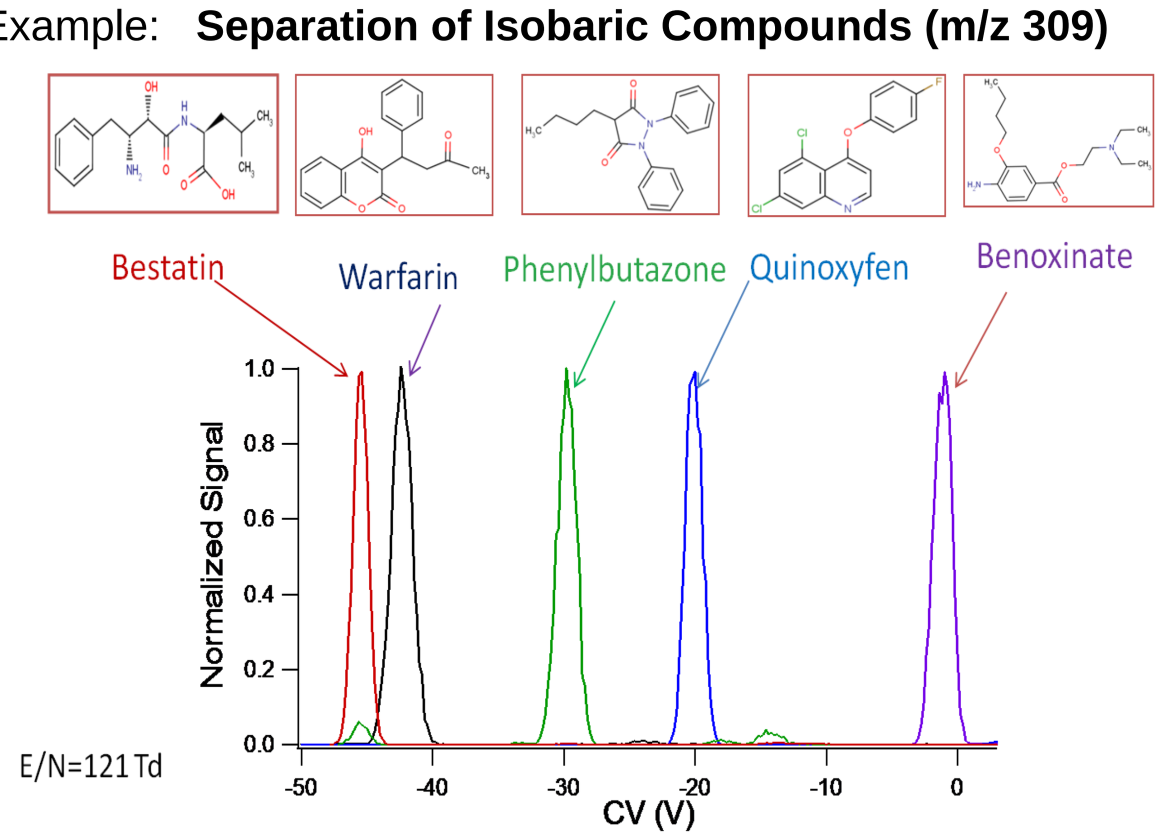
#3 Separation of stereoisomers, including diastereomers, and isobaric ions.

Example: **Separation of Ephedrine & Pseudoephedrine**



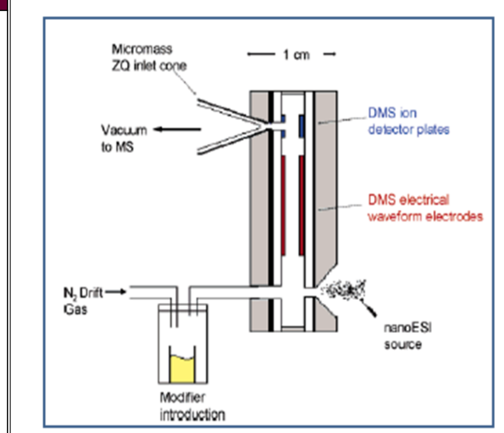
- Both chemicals have identical MW=165.11536, and almost the same structure.
- MS can not resolve these chemicals, DMS separates them.
- Decreasing flow rate helps improve separation, but in the same time decreased sensitivity.

Example: **Separation of Isobaric Compounds (m/z 309)**

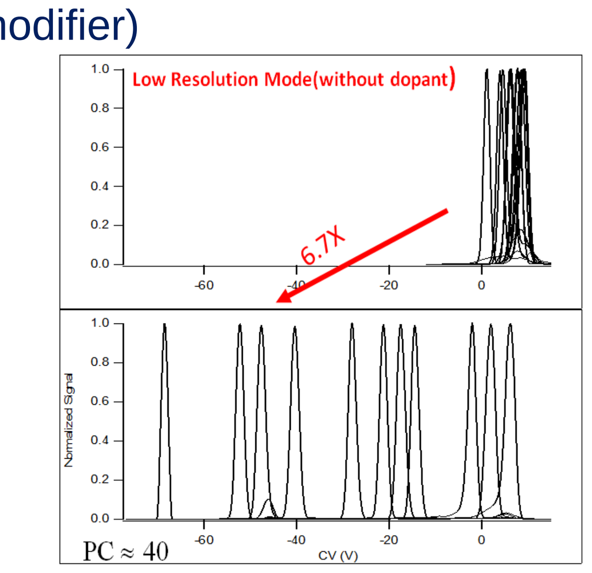


#4 Enhancement of resolution with chemical modifiers.

Example: Organic Chemical Modifiers for Enhancing Resolution . (2-propanol modifier)



Liquid modifiers such as 2-propanol can be added to our curtain gas flow.

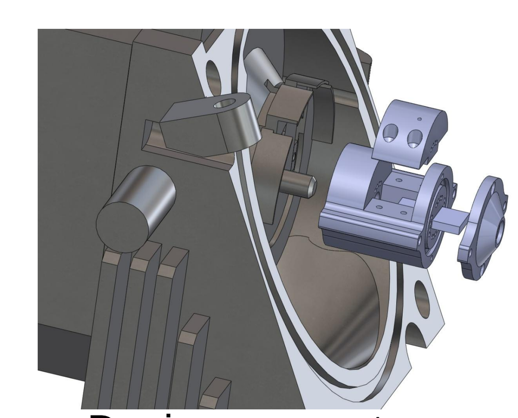


11 compounds: methylhistamine, minoxidil, ephedrine, norfentanyl, acyclovir, clenbuterol, tramadol, quinoxifen, pamaquin, fendiline, buscopan.

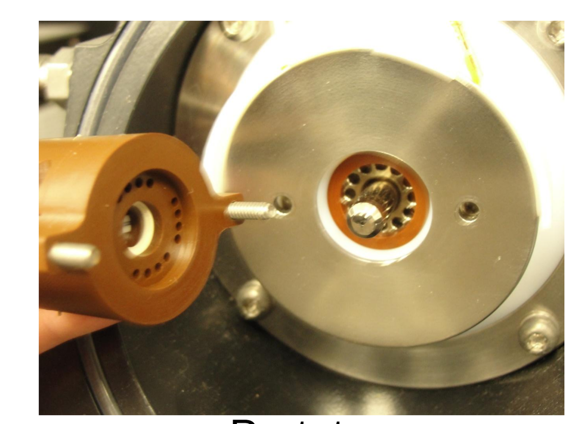
#5 Electromechanical simplicity, robustness. Rapid mounting and demounting of the interface.

New design interface for API MS with capillary inputs

Currently developed universal DMS interface design concept can operate with field–deployable and desktop type APIMS. Interface contains a planar DMS chip with chemically inert Vespel housing. Design provides electromechanical simplicity and robustness. Easy for install and uninstall with MS without breaking vacuum in analytical segments of MS.



Design concept



Prototype

Conclusions

A prototype of planar design of DMS interface for the atmospheric pressure ionization mass spectrometer with capillary inlet DMS pre-filtering has been designed and implemented.

•The combination of the two techniques substantially enhances the analytical power of the miniature MS; it increases its specificity and sensitivity in the analysis of complex mixtures.

Acknowledgements

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