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Dual Polarity Ion Confinement and Mobility Separations

Isaac K. Attah, Sandilya V.B. Garimella, Ian K. Webb, Gabe Nagy, Randolph V. Norheim, Colby E. Schimelfenig, Yehia M. Ibrahim[#], and Richard D. Smith[#]

Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA USA

Abstract

Here we present simulations and describe the initial implementation of a device capable of performing simultaneous ion mobility (IM) separations of positive and negative ions based upon the structures for lossless ion manipulations (SLIM). To achieve dual polarity ion confinement, the DC fields used for lateral confinement in previous SLIM were replaced with RF fields. Concurrent ion transport and mobility separation in the SLIM device are shown possible due to the nature of the traveling wave (TW) voltage profile which has potential minima at opposite sides of the wave for each ion polarity. We explored the potential for performing simultaneous IM separations of cations and anions over the same SLIM path and the impacts on the achievable IM resolution and resolving power. Initial results suggest comparable IM performance with previous single-polarity SLIM separations can be achieved. We also used ion trajectory simulations to investigate the capability to manipulate the spatial distributions of ion populations based on their polarities by biasing the RF fields and TW potentials on each SLIM surface so as to limit the interactions between opposite polarity ions.

Graphical Abstract

Keywords

Dual polarity mass spectrometry; Structures for lossless ion manipulations; SLIM; Ion Mobility

Introduction

The analysis of both positive and negative ions is important in a variety of applications due to sample and compound polarity-related variations in ionization efficiencies, fragmentation

[#] Corresponding authors: yehia.ibrahim@pnnl.gov and rds@pnnl.gov.

pathways, ion-molecule chemistries and ion mobilities. Currently, such measurements require switching of the DC voltages' polarity applied to the ion source, interface regions, and the MS. On the other hand, the time-averaged effects of time-varying waveforms, such as using radio frequency (RF) fields or traveling waves (TW), are largely agnostic to the polarity of ions in regard to their transmission or trapping.¹⁻³ The ability to study molecules in both positive and negative ion modes increases the information achievable, making MS more broadly applicable for complex samples and with different physicochemical properties. Although most biochemical MS analyses are routinely done in the positive ion mode, differences in molecular ionization efficiencies, suppression effects, and interferences can lead to loss of vital information. For example, while most peptide analyses are done in the positive ion mode, more acidic peptides and proteins (having relatively large numbers of acidic residues such as aspartic acid and glutamic acid), and several post-translationally modified peptides and protein are less effectively analyzed, and increased performance can often be achieved in the negative ion mode.⁴⁻⁸ Also, most lipidomics analyses are done in the negative ion mode as the lipids are often anionic or weakly anionic.⁹⁻¹⁴ However, some lipids are electrically neutral but polarizable and best suited for positive mode analysis. In general no single polarity MS analysis will be both broadly effective and sufficiently sensitive in the study of complex samples¹⁵⁻¹⁸, and there exists a need for more routinely conducting sample analyses in both positive and negative ion modes. This is particularly the case when samples become highly limited in size and are also unique (e.g. as in single cell analyses, tissue imaging, etc.), or when analyses would be ideally conducted simultaneously from the same sample.

Dual polarity sample analyses have very often been limited to separate single polarity measurements,^{13,19-22} or employ the use of polarity switching instruments with significant limitations on the speed of switching.^{13-15,23-25} Currently, simultaneous dual detections systems²⁶⁻³⁰ are generally limited to ionization under vacuum and e.g. the use of dual TOF MS systems, and thus have very limited utility. In contrast, separate single polarity analyses can be impractical as rapid polarity switching is technically challenging,^{24,27,31} due to ion source instability, subtle changes in experimental and instrumental conditions over time, overall low duty cycles, etc.^{24,28} The alternative approach of using two single-polarity power supply modules (or separate mass spectrometers) is similarly often impractical.^{13,18,32,33} True simultaneous dual polarity MS-based analytical instrumentation does not presently exist to the best of our knowledge.

In addition to MS, ion mobility (IM) spectrometry, where ions are separated based on their combined m/z and size/shape-based interactions with a buffer gas, is being increasingly utilized for analytical applications.³⁴⁻³⁶ IM has now been implemented based upon a range of approaches, e.g. drift tubes, traveling waves in stacked electrode ion guides, and FAIMS to name a few.³⁷⁻⁴⁰ Increased resolution makes IM increasingly useful,^{40,41} and its utility independent of the MS analyzer also proportionally increases.

In this context, our laboratory has been developing a new approach for IM-based separations based upon Structures for Lossless Ion Manipulations (SLIM) that has already demonstrated large gains in IM separation resolution and other aspects of performance.⁴²⁻⁵³ SLIM-based design implementations using traveling waves (TW) have provided the ability to achieve

exceptionally long IM path lengths and thus increased resolution without the need for the higher voltages that would be required e.g. for extending the length of IM drift tube designs.^{43,44,46} SLIM serpentine ultra-long path with extended routing (SUPER) multi-pass implementations have been shown to provide ultra-high resolution for targeted IM ranges in the analysis of complex samples with MS.^{43,44,51} The flexibility in electrode arrangements and the generated electric fields for manipulating ions offered by SLIM has also enabled the accumulation of much larger ion populations than previously feasible, providing the basis for e.g. and enhanced sensitivity for analysis of low abundance species.^{43,44,51–53} In this regard, the development of TW-based SLIM compression ratio ion mobility programming (CRIMP)⁴⁵ has been shown to allow initially broad ion distributions (and IM peak widths) to be minimized after an initial period of separation to relax space charge effects, and provided the basis for effective use of these large ion populations in subsequent ultra-high resolution IM separations. CRIMP has also shown utility for mitigating the undesirable effects of diffusional broadening and the initial ion spatial distribution on IM resolution, reducing peak widths and increasing peak intensities (and S/N) in SLIM IM separations without significant impact upon IM resolution.

Here, we describe the development of a SLIM device capable of performing simultaneous positive and negative IM separations in the same ion path as part of an effort to develop a dual polarity IM spectrometry platform.

Experimental Setup

Agilent low concentration ESI tuning mixture (Agilent, Santa Clara, CA) was infused at a flow rate of 0.3 $\mu\text{L}/\text{min}$ and ionized to form singly charged phosphazine ions in either positive or negative polarity modes by nanoelectrospray ionization (± 2500 V) for analysis using a SLIM IM Q-TOF MS (Figure 1). In this work ions were introduced through a 500 μm i.d. stainless steel capillary heated to 120 $^{\circ}\text{C}$ which had an applied voltage of 350 V for positive ion analysis and - 350 V for the negative ion, and then entered an ion funnel (1.0 MHz, ~ 200 V_{pp} and 3.9 Torr) with the gradient voltages set to reflect the polarity of the ions being analyzed. In the absence of a pulsed trapping or accumulation region, such as an ion funnel trap^{54,55}, ions were injected to the SLIM module for 3 ms by pulsing the voltage applied to the conductance-limiting (bottom) lens (2.5 mm i.d.) at the exit of the ion funnel. The SLIM chamber was filled with ultra-high purity nitrogen (4.0 Torr) and the pressure was monitored using a convectron gauge (Granville-Phillips, Boulder, CO). The arrays of TW electrodes of the SLIM module used in this work had a 2.0 mm length and 0.5 mm width, with ~ 0.10 mm gaps between all electrodes. The RF electrodes on the SLIM module had a width of 0.5 mm while the guard electrodes have a width of 3.0 mm. The SLIM module had a total path length of 90 cm, and the spacing between the two SLIM surfaces was 3.2 mm. Ions exit the SLIM module into a 15 cm long rear ion funnel (0.8 MHz and ~ 120 V_{pp}) and then transferred through a differentially pumped region (400 mTorr) using a short quadrupole (2.3 cm long, 6.4 mm diameter, and 2.8 mm inscribed radius). Ions are then transmitted for detection to an Agilent QTOF MS equipped with a 1.5 m flight tube (Model 6538). In this work the polarity for all ion lenses except in the SLIM module were set with respect to the polarity of ions being analyzed. Polarity switching of the confinement and transmission lenses of the instrumental setup used in this study was necessary since the

instrument is designed to confine and transmit ions of only one polarity at a given instance. The lenses included the ion funnels just before and after the SLIM device, and all the ion optics of the Agilent QTOF.

Ion trajectory simulations were done using SIMION 8.1 (Scientific Instrument Services, Ringoes, USA). The geometry of the SLIM device was first built in SolidWorks CAD software (Dassault Systems Solidworks Corporation, Waltham, MA) and then imported into SIMION, and the respective electrode voltages assigned. The SLIM device was 32.0 cm long, with a gap of 3.0 mm between the two SLIM surfaces. The TW electrodes were 2.0 mm in length, and 0.5 mm in width. The RF electrodes on the board surfaces were 0.5 mm in width. The guard electrodes had a width of 3.0 mm. The potential arrays were generated by using the refine feature in SIMION, with a convergence criterion of 0.001. The workbench for simulations was controlled using an in-house Lua programming code compatible with SIMION. Details on the signals applied to the respective electrodes are discussed below. An SDS model was used to simulate ion- nitrogen buffer gas collisions at 4.0 Torr pressure.^{56,57} Ions are presumed to have zero initial kinetic energy, and space charge effects were ignored in these trajectory simulations. To generate the pseudo-potential energy contour plots, both the fields generated by the applied RF on all the RF electrodes and the DC potentials from the TW applied were extracted using the “STL to text file” feature in SIMION. The composite pseudo-potential images were then processed by superimposing the two profiles using an in-house Matlab code. For ion statistics, 250 positive ions and 250 negative ions each for every m/z considered (Table 1) were used to simulate the transmission efficiency of the new SLIM device. 1000 positive ions and 1000 negative ions each for m/z 622 and m/z 922 was used to simulate the resolution and resolving power reported here.

Results

The electric potentials and fields created for ion confinement and manipulation in SLIM have been previously reported in conjunction with the development of SLIM-based technology.^{46–50,52,53} Figure 2a shows a schematic diagram of the present SLIM configuration, illustrating 2 sets of the 3 arrays of 8 TW electrodes sequence sets interspaced by the 4 extended electrodes (i.e. a 4,3 arrangement⁵⁸) on which the RF potentials are applied (with opposite polarity to adjacent RF electrodes). Transient DC voltages are applied to the TW electrodes in a given sequence to create the repeating dynamic voltage wave profile that is used for ion manipulation. Figure 2b shows a ‘4 up-4 down’ TW sequence (i.e. HHHHLLLL) in which the 4 electrodes in the H state have a higher (or positive) DC potential applied, forming the TW maxima, and 4 electrodes in the L state have the lower (or negative) potentials applied, creating the TW minima. The wave is propagated by changing (with a given frequency) selected electrodes from H to L or L to H in a stepped fashion; e.g. the first electrode in each array of 8 goes to L and a higher DC (H) is applied to the fifth electrode in each array. In the next time step, the first and the second electrodes have L applied while the fifth and the sixth have H applied. The repetition of this process over all the arrays of 8 electrode sequences creates a moving wave, as shown in Figure 2c. Figure 2d shows a representation of the 2 parallel SLIM surfaces separated by a 3.2 mm gap, as used in this study.

Our earlier SLIM implementations used static DC potentials applied to ‘guard’ electrodes to provide lateral confinement (i.e. in the XZ direction) in conjunction with the RF fields applied to the RF electrodes on each SLIM surface that create pseudopotentials that prevents ions from closely approaching either surface. However, any simultaneous dual ion polarity design requires the elimination of all elements that will lead to the loss of ions of one polarity, and specifically the DC guard electrodes. Figure 3a shows a schematic of the modified SLIM module that was optimized here to successfully confine both positive and negative ions using the same effective potentials and field conditions. This design used guard electrodes to which RF potentials are applied in place of static DC potentials. The two guard electrodes for each SLIM surface that define an ion pathway have the opposite phases applied RF with respect to each other to create a potential barrier in the lateral dimension. The RF potentials applied to the RF electrode strips on each surface used a somewhat lower amplitude but the same frequency as the guard electrodes, and were configured to have the same RF phase on the outer most RF electrodes and their adjacent guard electrodes. Figures 3b and 3c show the effective potential contour plots illustrating the design’s effectiveness for confining ions of both polarities. Effective fields were calculated using the fast-adjust function in SIMION and processed using an in-house Matlab (Mathworks, Natick, MA, USA) code. The effective potential calculations used the superimposed RF and transient TW potentials applied to the SLIM electrodes. Under the same simulated conditions (TW: 45 V_{pp} at 200 m/s, TW sequence: LLHHHHLL, RF_{electrode}: 310 V_{pp} at 0.8 MHz, RF_{guard}: 360 V_{pp} at 1.0 MHz), a cation of m/z 622 experiences the lowest confining potential in the center of the device in the YZ plane, with the fields becoming greater away from the center. Importantly, an anion of m/z 622 is also observed to experience a similar potential under the same SLIM conditions, where the bottom of the confining potential well also lies in the center of the YZ plane. The overall confining fields in this RF-guard SLIM are observed to be highly quadrupolar (Figures 3b and 3c). The average velocity of an ion as it travels through the SLIM device, at a given background gas pressure, is dependent on its mobility. For a given TW velocity, if the ion’s mobility is sufficient to allow a velocity that is greater or equal to the TW velocity, the ion will keep up with the TW as it travels (i.e. ‘surf’, or moves in the ‘traveling traps’). If their mobility is insufficient ions will be passed over periodically by waves, falling into the potential trough of a following wave. The lower their mobility, the more frequently it will be passed by waves, and the more slowly it moves on average.

An important difference between the motions of anions and cations is due to the position of the TW maxima and minima (Figures 3b and 3c), and where ions of each polarity are expected to spend most of their time in spatially separated traveling traps. The cations will experience the TW minima (i.e. the wave trough) in the TW profile L state, anions in the H state (as previously described in Figure 2b). As a result, most of the time cations and anions will not occupy the same physical space, spending most of their time in their different wave troughs.⁴⁸ However, in the IM separation mode, ions do not stay in the minima as they roll over a passing wave, and lower mobility ions of opposite polarity will have a higher probability of interaction. An approach for the control of such potential ion-ion interactions in the separation mode will be discussed later.

To assess the potential IM performance, simulated IM data was generated using SIMION for the new SLIM design and compared to a SLIM configuration using previously published experimental data.^{49,58} SIMION successfully reproduced the published data, supporting the utility of our simulation model.^{45,47,57,59} Figure 4 shows simulated arrival time distributions (ATDs) and nested mass spectra for positive and negative ions of m/z 50 to 3500 using the 32 cm long dual-polarity SLIM. A list of the ions used and their reduced mobilities is given in Table 1. Figure 5a shows the simulated transmission efficiency for ions of both polarities. The top half of the figure shows the ions of m/z 50–3500 being transmitted through the SLIM with 15 V DC applied on the guard electrodes. With the exception of the lowest m/z (50) (for which effective confinement is not expected with the present RF frequency and 4 Torr of N₂ buffer gas), all cations were successfully transmitted in these simulations, whereas all negative ions were lost (to the guard electrode). In the lower half of Figure 5a, shows that application of RF (360 V_{pp} at 1.0 MHz) to the guard electrodes in place of a static (15 V) DC potential results in the transmission of all cations and anions ions, again with the exception of 50 m/z ions. Figure 5b shows the theoretical resolution from simulations for the m/z 622 and m/z 922 ions of both polarities as a function of TW speed. We observe that the resolution provided by the two SLIM designs (green trace for the DC guard SLIM, and black trace for RF guard SLIM) decreased in a similar manner. Another measure of performance is the IM resolving power using the m/z 622 ion using the new RF guard SLIM module. Similarly, Figure 5c shows the m/z 622 cation and anion theoretical resolving power, for both the DC guard SLIM (green) and the RF guard SLIM (black), increases as the TW speed increases to ~150 m/s and then starts to decrease at higher TW speeds. Collectively, these simulations indicate that similar performance can be expected for the SLIM RF guard and the DC guard designs.⁴⁹

The spatial distributions of cations and anions

Confined ions have the highest probability of residing in an effective ‘ion conduit’ defined by the RF effective potentials (i.e. where they experience the least repulsive effective potential), near the middle of the SLIM ion pathway. However, perturbations due to space charge, field penetration from other regions, etc., may impact ion spatial distributions. Figure 6a shows the arrangement used in simulations discussed below for a gap of 3 mm between the two SLIM surfaces. Figure 6b shows that the singly charged cations and anions (black and blue for positively charged m/z 922 and m/z 1522 ions; red and green for negatively charged m/z 922 and m/z 1522 ions, respectively) indeed occupy space towards the center of the SLIM ion pathway. Although we expect that effective field-free regions can be incorporated into similar SLIM designs that would facilitate increased ion-ion interactions, if desired, generally we anticipate that simultaneous dual polarity IM analyses would benefit from cations and anions being physically separated to prevent losses due to reactions (e.g. neutralization, charge transfer).^{48,60–63} As noted earlier, there is an axial displacement of different ion polarities due to the TW, such that ions of different polarity and high mobility that are moving with the wave (i.e. surfing) will not interact; ions of increasingly lower mobility (that are being separated) will experience increasing interactions. Ion-ion interactions have increased probability for occurring as the relative velocity of the positively and negatively charged ion approaches zero. Under conditions

where lower mobility species will undergo separation, a cation and an anion in the SLIM device could potentially interact every time they roll over a passing wave. The critical distance, the minimum distance between the two ions at which point they have the highest probability to form an orbit bound ion complex, has been estimated to be 162 μm at a relative velocity of 2 m/s,⁴⁸ and to avoid possible interactions the separation between these two species should ideally be significantly greater. A bias voltage applied to one SLIM surface can move ions of opposite polarity into regions closer to the other surface. This is illustrated in Figure 6c, which shows the ions separated into two distinct ion populations based on their respective polarities after a bias voltage of 8 V (4 V on one SLIM surface, and -4 V on the other SLIM surface) was applied to across the SLIM device. The separation between the two polarities is ~ 0.6 mm, which is ~ 3.7 times larger than the calculated critical distance reported for a singly charged anion and cation under separations conditions, moving at relative speeds of 2 m/s.⁴⁸ The probability of ion-ion interactions in the SLIM is expected to be minimal, as under separation conditions the relative velocity of a cation and an anion (both of 622 m/z and a Ko of 1.17cm²/Vs) was calculated to be less than 3 m/s for $\sim 2.5\%$ of the total ion separation time.⁴⁸ This ratio, however, is expected to increase for larger ions with lower ion mobilities. Further ion parsing can be achieved by increasing the bias voltage across the SLIM device, as shown in Figure 6d. However, excessive bias across the SLIM device will displace ions into regions of higher RF fields, leading to increasing ion activation. To evaluate the effect of biasing the RF guard SLIM device on its IM performance, the performance criteria discussed above were repeated with a 6 V bias applied between the SLIM surfaces. Figure 7a shows the simulated transmission efficiency of 250 positive ions and 250 negative ions each for every m/z used in this study (Table 1) through a 32 cm long SLIM pathway. When a 6 V bias is applied across the SLIM device, somewhat reduced transmission ranges were observed (top) compared to the efficient transmission for all ions $>m/z$ 50 without bias applied (bottom). However, we note that the simulations indicate the resolution and resolving power is similar to without bias applied (Figure 7b and c).

Initial experimental ion mobility performance

This work provides a foundation for the development of an instrument having the capability to simultaneously analyze anions and cations. This undertaking requires the modification of approaches designed for single-polarity ion transmission or confinement. One challenge with dual polarity mass spectrometry is with sample ionization. It is well established that solvents or solutions of different compositions may be needed to provide desired ionization efficiencies for either positive or negative ion mode ionization, respectively, for the analysis of the same analyte.^{64–67} One possible approach to overcome the complexity of ionization owing to the choice of solvent/solution is the utilization of neutral or voltage free spray ionization techniques. A few such techniques are Sonic Spray Ionization,⁶⁸ Desorption Sonic Spray Ionization,⁶⁹ Zero Volt Paper Spray Ionization,⁷⁰ Surface Acoustic Wave Nebulization,⁷¹ among others. In this work, Agilent tune mix which was used to assess the performance of the SLIM device, is well known to ionize efficiently in both ion polarity modes. In future work where we hope to ionize more complex and diverse samples, a

practical approach to this problem is to have two separate ESI emitters and capillaries for the ionization and introduction of positive and negative ions respectively.⁷²

Guided by results from ion simulations we fabricated a dual polarity SLIM for initial evaluation in conjunction with an Agilent QTOF MS, which can be operated in either positive or negative polarity mode (but not simultaneously). Figure 8 shows the arrival time IM-MS spectrum collected for Agilent low concentration tune mix using the same SLIM parameters for both measurements. In Figure 8a, cations were analyzed with the MS operated in the positive ion mode, and in Figure 8b, anions from the same sample were analyzed with the MS operated in the negative ion mode. The results indicate that the dual polarity SLIM functions efficiently for ions of opposite polarity simultaneously. In figure 8a, the cutoff for the higher m/z ions, which also corresponds to the lower mobility ions observed, is compared to the wider transmission range observed for the negative ion spectra in figure 8b. This observation can be attributed positive mode tuning for the Agilent TOF MS used in this experiment (the observation was consistent with our experience for the positive mode with this Agilent TOF MS)^{49,58}. Similar performance has been observed in the positive mode for this Agilent QTOF MS.^{49,58} While mobility separation of both ion polarities can be done simultaneously the resolution was not optimized in this initial work which used a broad initial ion packet. Future work will explore the dual polarity SLIM switch and also to enable simultaneous dual polarity ion current measurements using two charge detectors in a stand-alone (without a mass spectrometer); a step towards a high resolution and high selective IMS instrument to explore potential for unambiguous molecular identification without the need for a mass spectrometer.

Finally, we note that the redesign or alternative operation will be needed for some upstream and downstream components to realize the full potential of the present developments, and we anticipate that full simultaneous IM-MS analyses should be feasible using e.g. simultaneous positive and negative mode electrosprays and ion funnels operated without DC potential gradients (using source derived gas flows), or the use of traveling waves. Similarly, traveling waves in conjunction with ion guides can be used to transmit ions in lower-pressure/vacuum regions to ion trap-based mass spectrometers where simultaneous dual detection is feasible.

Conclusions

We report a dual ion polarity instrument capable of performing simultaneous manipulations, including IM separations of both cations and anions, and a major step towards IM-MS instrumentation capable of performing simultaneous positive and negative ion analyses. We have shown initial experimental data demonstrating IM separations in the new SLIM design for cations and anions without changing the TW or other SLIM parameters. The performance of the new SLIM module has been assessed using simulations, and it is predicted to perform similarly to the conventional TW-based SLIM (i.e. using DC-only guard electrode potentials). These results highlight not only the potential of SLIM for dual polarity analyses, but also its general utility as a platform for ion manipulations that include ion-ion interactions and where ions of both polarities are desired to be simultaneously, and ideally efficiently, manipulated.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

Acknowledgments

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Figure 1.

Schematic of the instrument setup used in this work, showing the TW SLIM device coupled to an Agilent 6538 QTOF mass spectrometer. The SLIM device in the setup was 90.0 cm long, with a gap of 3.0 mm between the 2 SLIM surfaces. The TW electrodes were 2.0 mm in length, and 0.5 mm in width. The RF electrodes and guard electrodes were 0.5 mm and 3.0 mm in width respectively.

Figure 2.

(a) Schematic diagram of a section of the SLIM module showing the layout of electrodes used to generate the fields; (b) illustration showing the programmable TW sequence used to generate the TW profile for ion manipulation and transport; (c) illustration of travelling wave propagation through the SLIM device achieved by stepping the programmed TW sequence in single electrode steps at a predefined speed; and (d) 3-D schematic of the arrangement of the 2 parallel SLIM surfaces (spacing not to scale) used for ion confinement and manipulation.

Figure 3.

(a) SLIM RF guard configuration optimized for dual ion polarity confinement and transport. The blue and red indicates the electrodes have two different phases of the RF phases applied (red for positive phase, blue for negative phase; shifted by 180 degrees). The black traces have TW potentials only applied. Effective potential contour plots were generated using SIMION by superimposing the RF fields on the DC potential of the traveling wave, generated separately in SIMION, and superimposed using MATLAB. The TW potential sequence was operated in a 'four up-four down' TW profile (e.g.: LLHHHLL) for each 8 electrode array sequence. (b) The effective potential experienced by a cation, m/z 622; and (c) the effective potential experienced by an anion, m/z 622. The top sections of Figures 3b and 3c show the effective potential view generated at the 4.6 mm from the start of the SLIM surface, as the ions travels in the YZ direction (elevation multiview). The lower sections of Figures 3b and 3c show the effective potential view generated at the 1.0 mm distance off the surface of the top SLIM surface, as the ion travels in the XY plane (plan view).

Figure 4.

(a) Simulated ATDs for positive ions (black) and negative ions (red) through the SLIM using RF guards. The inset shows the simulated ATDs for positive ions as a function of m/z ; a similar distribution was obtained for negative ions.

Figure 5.

(a) Transmission of positive and negative ions (m/z 50 – 3500) with DC guards (top) and RF Guards (bottom), respectively; (b) mobility resolution for the m/z 622 and 922 peaks; and (c) resolving power for m/z 622. Similar transmission was observed for 84 m/s and 400 m/s.

Figure 6.

(a) Arrangement of the two SLIM surfaces and the direction of ion motion used for simulations of ion trajectories between the SLIM surfaces as a function of bias voltage applied for singly charged cations and anions (black and blue for positively charged m/z 922 and m/z 1522 ions; red and green for negatively charged m/z 922 and m/z 1522 ions, respectively); (b) no bias voltage applied; (c) 8 V (+4 V on the top surface, and -4 V on the bottom surface) bias applied; and (d) 20 V (+10 V and -10 V) bias applied. Figures 6b to 6d each show a 1 cm long section of the 32 cm long SLIM device used in this SIMION simulation (position 16 cm to 17 cm). The starting and end position of the ions not shown in the figures.

Figure 7.

(a) Plot showing the transmission efficiencies of positive and negative ions (m/z 50 – 3500) with the RF guard a 6V surface bias (top) and with no surface bias (bottom), respectively, as a function of m/z ; (b) resolution for the m/z 622 and 922 peaks; and (c) resolving power for m/z 622. Similar transmission performance was observed for 84 m/s and 400 m/s. The lower panel of figure 7a, along with the black and red traces in Figures 7b and 7c (Positive Ions_RF Gurad_No Bias and Negative Ions_RF Gurad_No Bias respectively) are repeated from figure 5 for comparison.

Figure 8:

Nested mass spectrum and time for the analysis of Agilent Tune Mix using the RF guard SLIM design in (a) positive ion polarity mode and (b) negative ion polarity mode. The SLIM parameters used were identical for both ion polarities

Table 1:

Mass and reduced mobilities (the same for both polarities) of ions used in the SIMION simulation. Reduced mobilities were generated from a fit to experimental measurements for Agilent tune mix ions.

Ion mass (Da)	Reduced mobilities (Ko, cm ² /Vs)
50	4.32
80	3.38
100	3.02
130	2.63
150	2.44
190	2.16
200	2.11
322	1.65
622	1.17
922	0.95
1222	0.82
1522	0.74
1822	0.67
2122	0.62
2422	0.58
2722	0.54
3000	0.52
3300	0.49
3500	0.48