



# Fundamentals of Ion Dynamics in Structures for Lossless Ion Manipulations

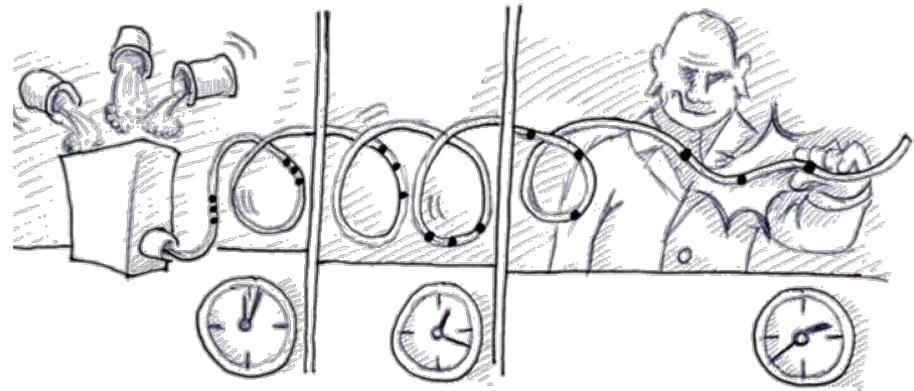
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# Separations prior to MS

## ○ Liquid chromatography separations

- liquid phase
- high performance
- packing material molecule specific
- slower



## ○ Ion mobility separations

- Gas phase
- fast
- broad applicability
- limited peak capacity

# Separations prior to MS

We need

Fast Separations

< 1s

# Separations prior to MS

We need

Fast Separations



High Resolution

< 1s

Long paths > 1m

# Separations prior to MS

We need

Fast Separations



High Resolution



High Sensitivity

< 1s

Long paths > 1m

Lossless

# Separations prior to MS

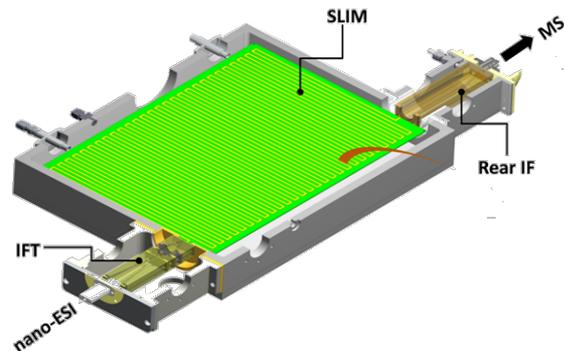
Fast Separations



High Resolution



High Sensitivity

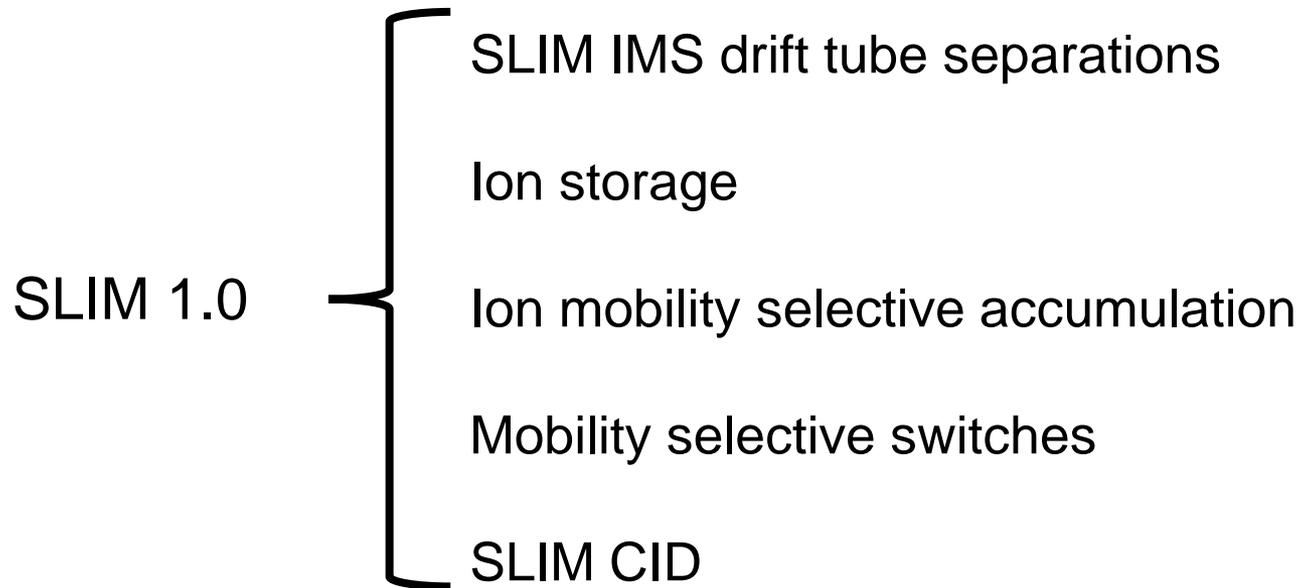


# Structures for Lossless Ion Manipulations

- Planar surfaces with electrodes to losslessly confine and manipulate ions

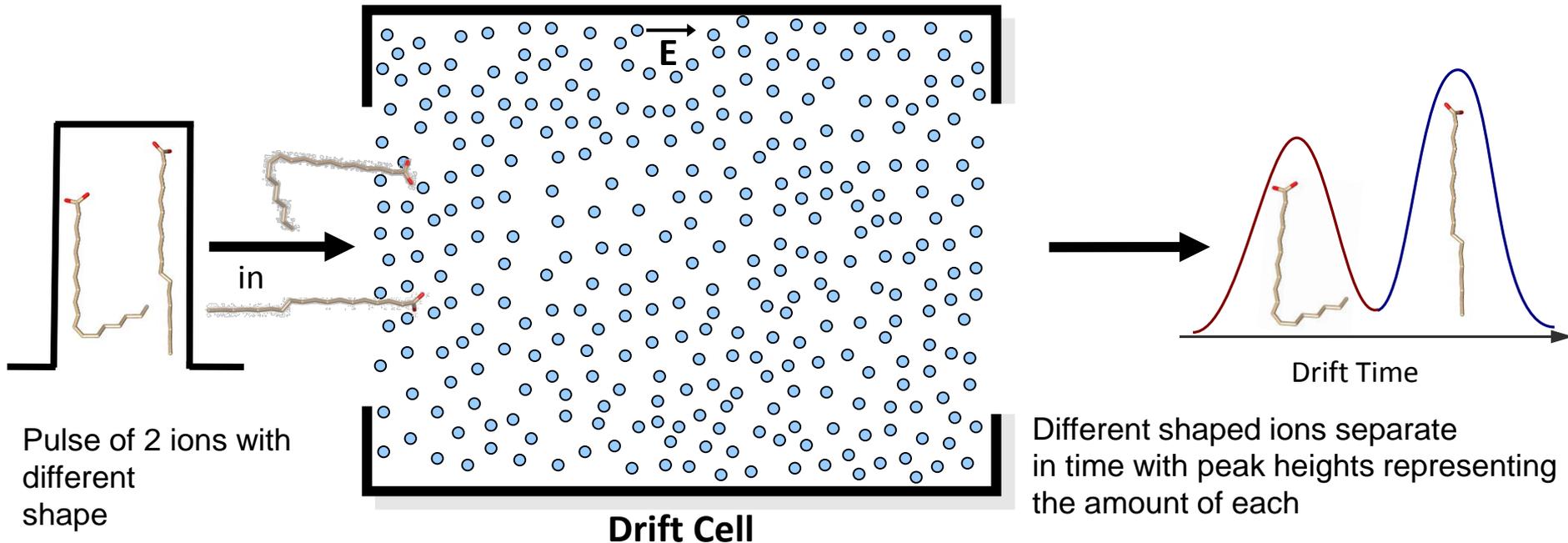
# Structures for Lossless Ion Manipulations

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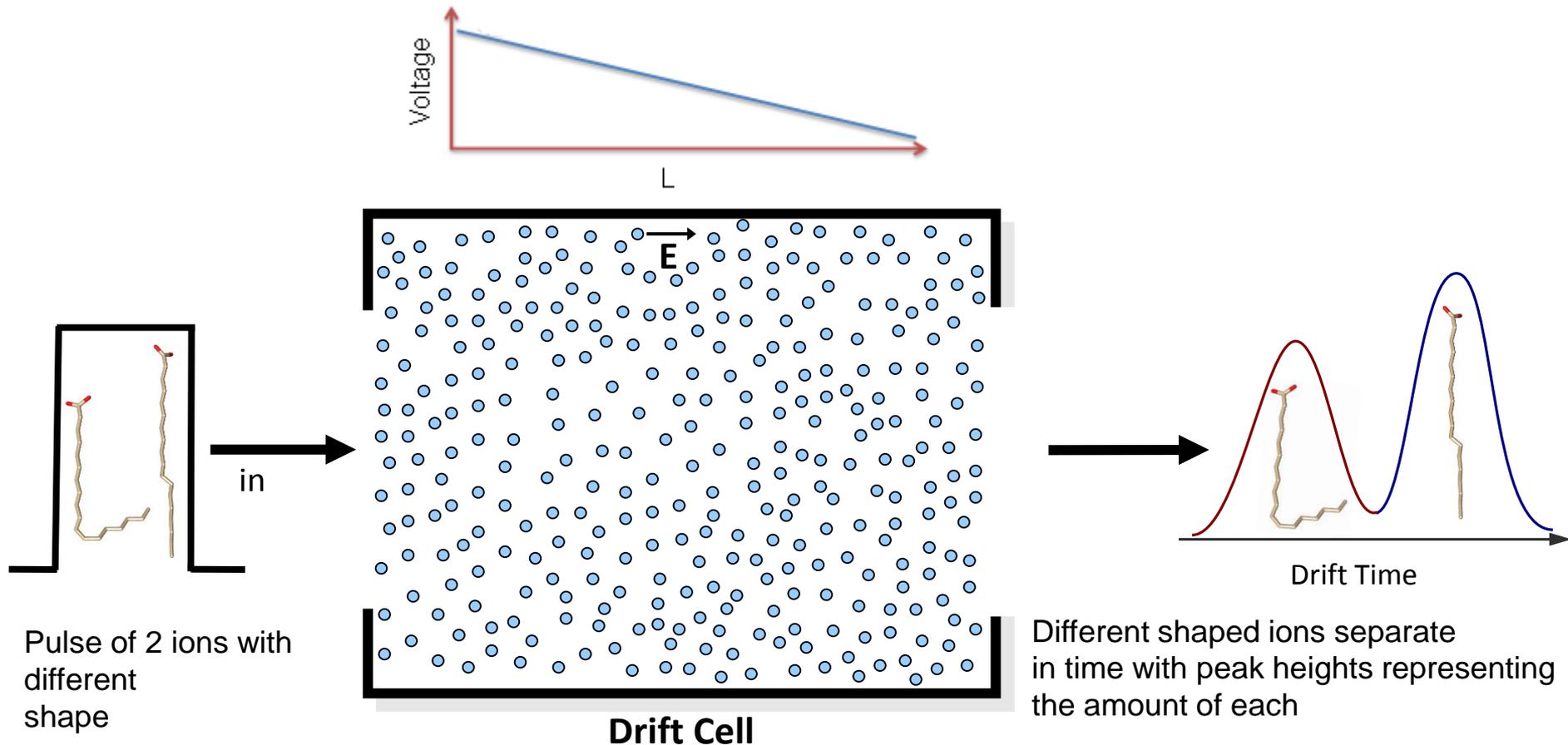
# Ion mobility spectrometry (IMS)

- Gas phase separation technique based on ion shape (i.e. collision cross section; CCS)
- IMS is a very fast separation technique which provides structural information
- IMS-MS, in conjunction with LC, has potential to greatly improved separations e.g. for analysis of complex samples



# Ion mobility spectrometry (IMS)

- Factors affecting IMS separations performance:
  - a) Separation path length
  - b) Temperature
  - c) Pressure



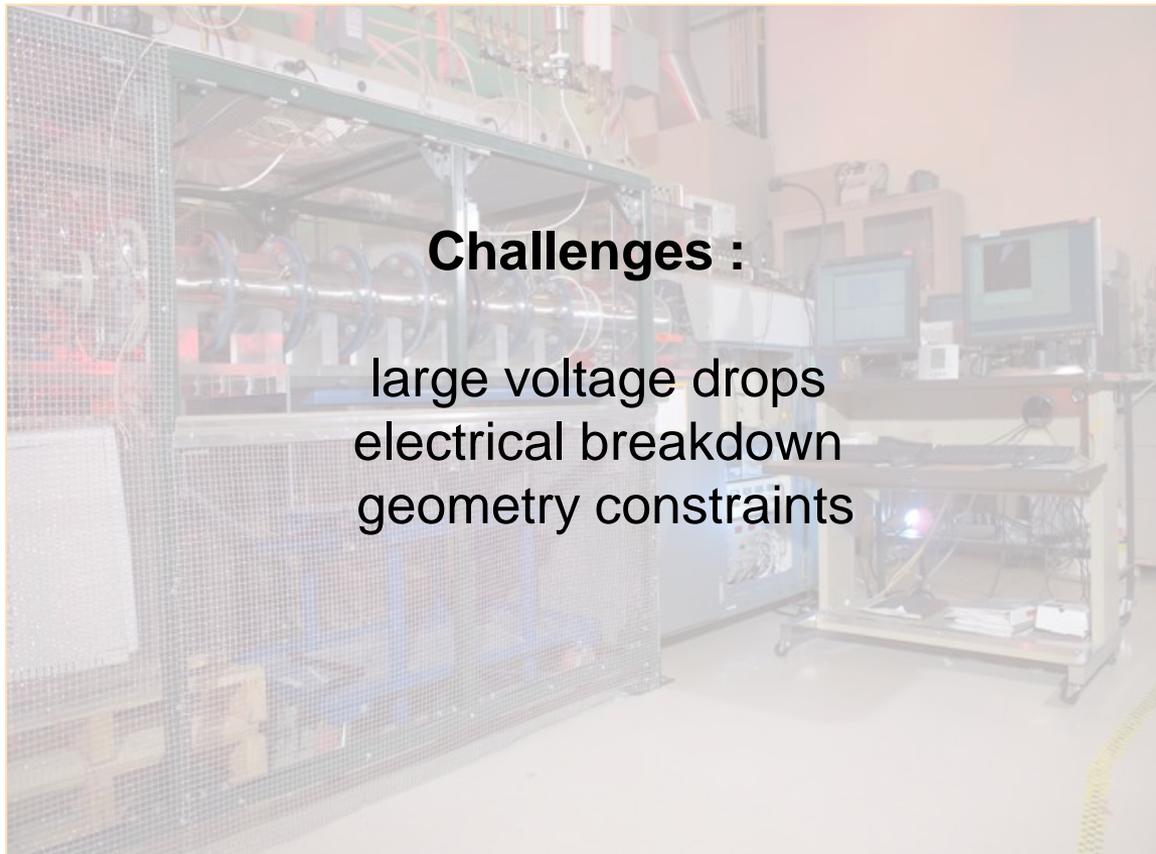
# Ion mobility spectrometry (IMS)

- Everything else being equal, IMS separations improved by increasing voltage drop (Longer path length or higher electric field)



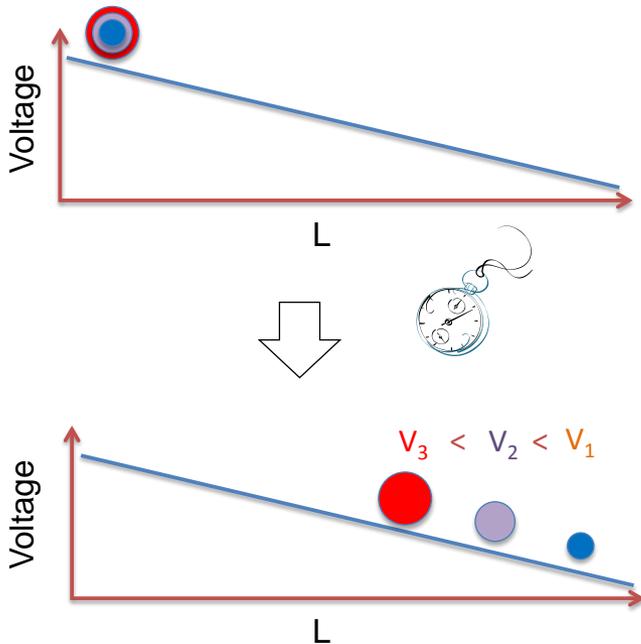
# Ion mobility spectrometry (IMS)

- Conventional drift tube separations improved by using:
  - a) Greater voltage drop (Longer path length or higher electric field)
  - b) Lower temperature



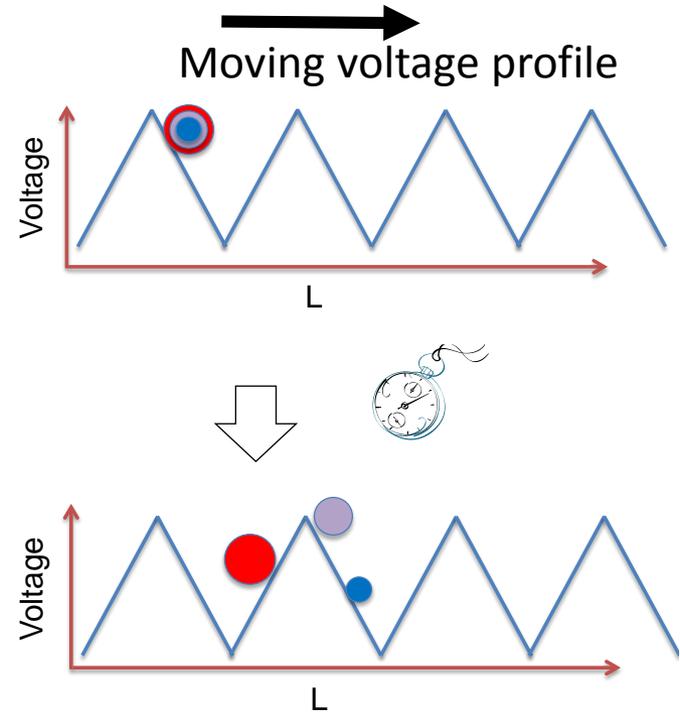
# Traveling wave IMS

## Drift Tube IMS



Voltage drop increases with drift length

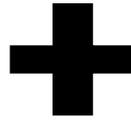
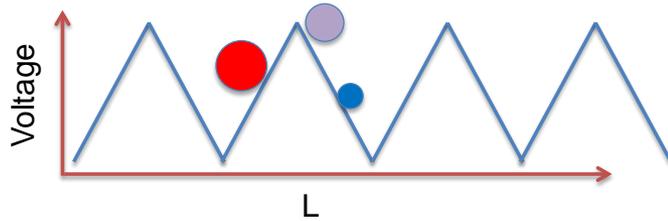
## Traveling Wave IMS



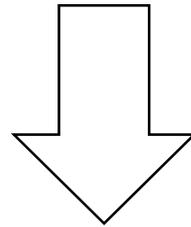
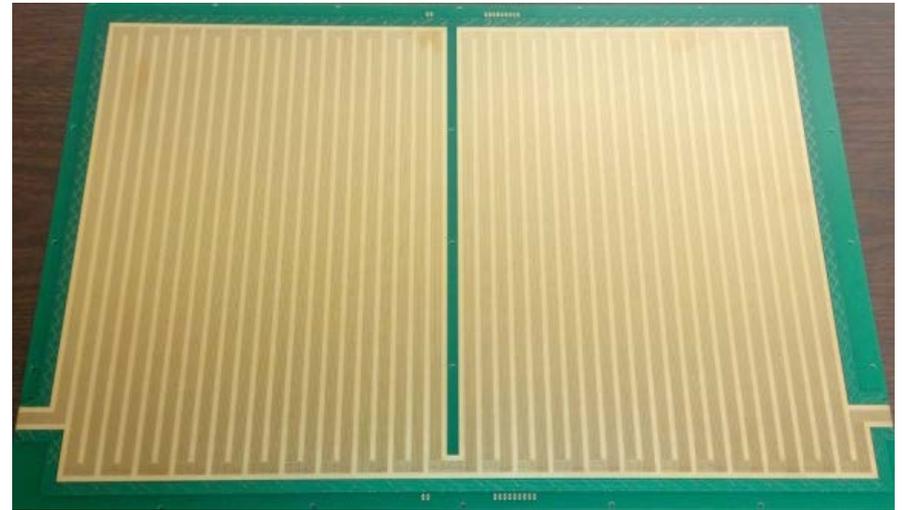
Fixed voltage profile moves along the total drift length

# TW-SLIM

TRAVELING WAVE SEPARATION

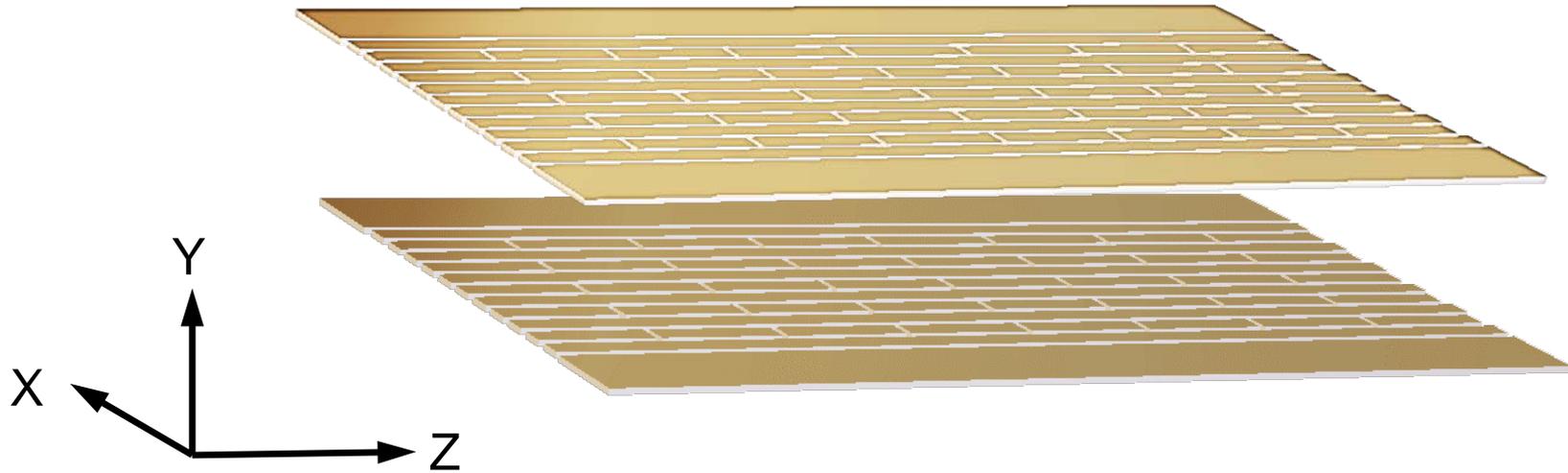


SLIM DEVICES



Very high resolution IMS separations

# SLIM 2.0 electrode arrangements for ion manipulation

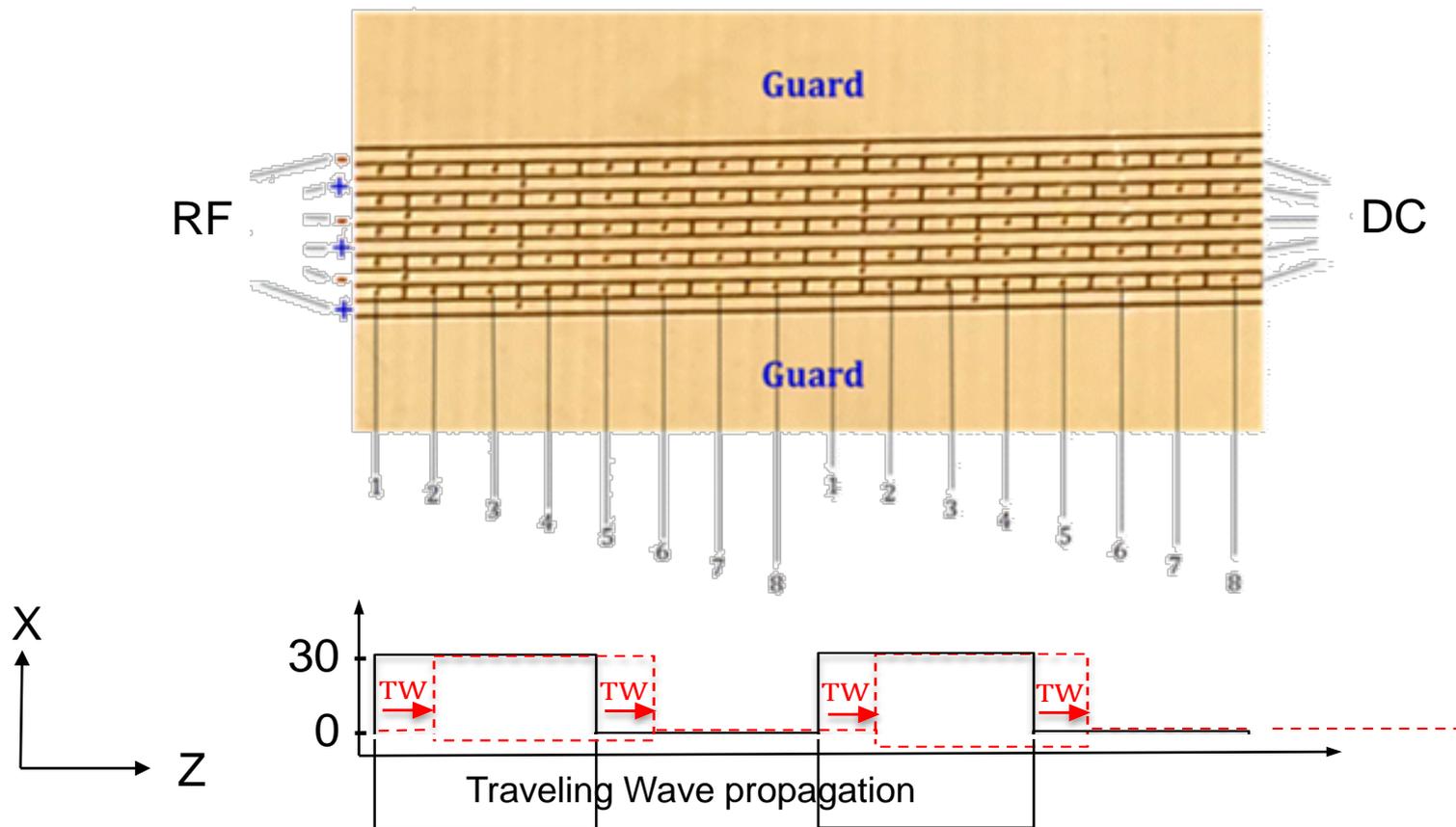


Two parallel surfaces

Each surface has electrodes

Distance between surfaces  $\sim 3$  mm

# SLIM 2.0 electrode arrangements for ion manipulation



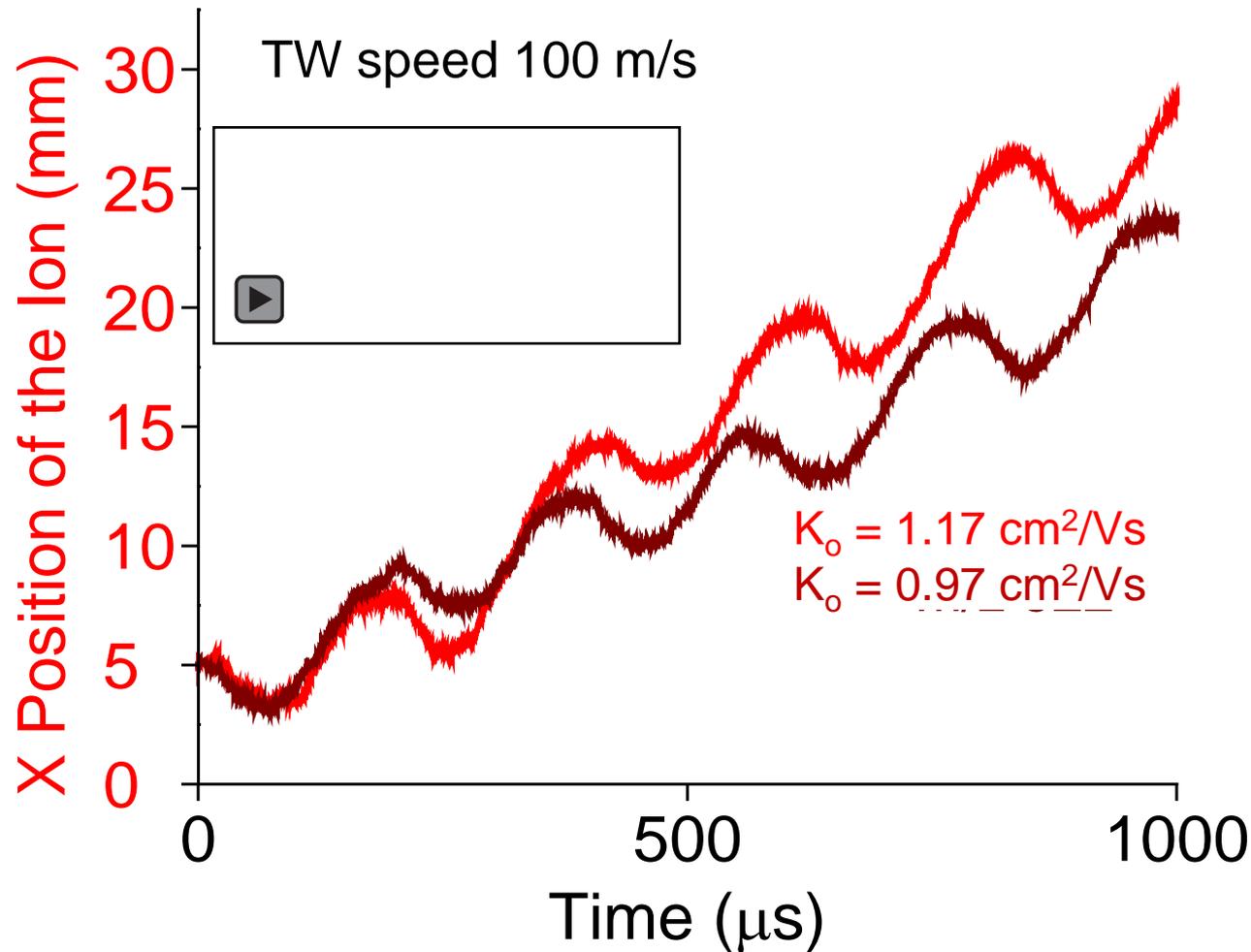
RF strip electrodes to enable ion confinement  
DC electrodes for applying traveling wave  
DC voltage profile steps forward at a fixed speed

# Separations mechanism in TW-SLIM

TW speed 100 m/s

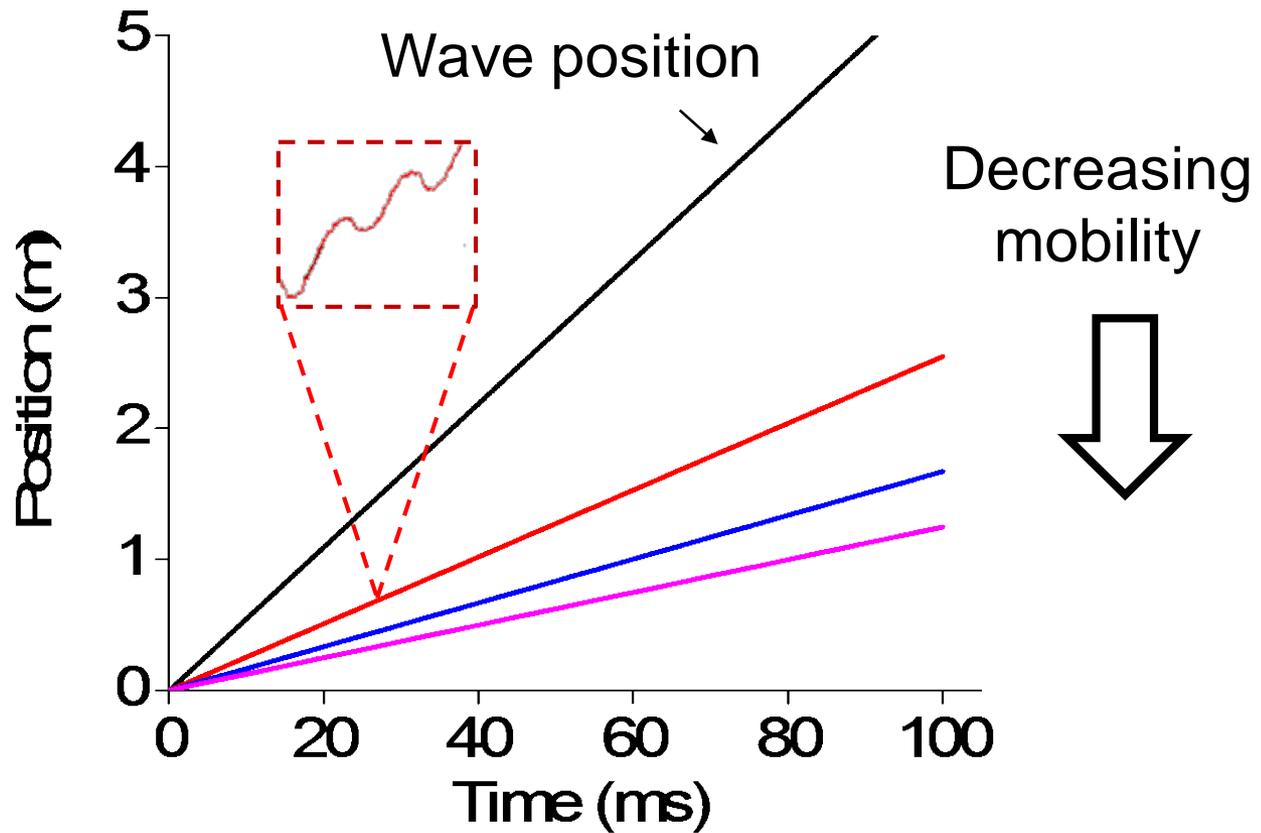


# Separations mechanism in TW-SLIM



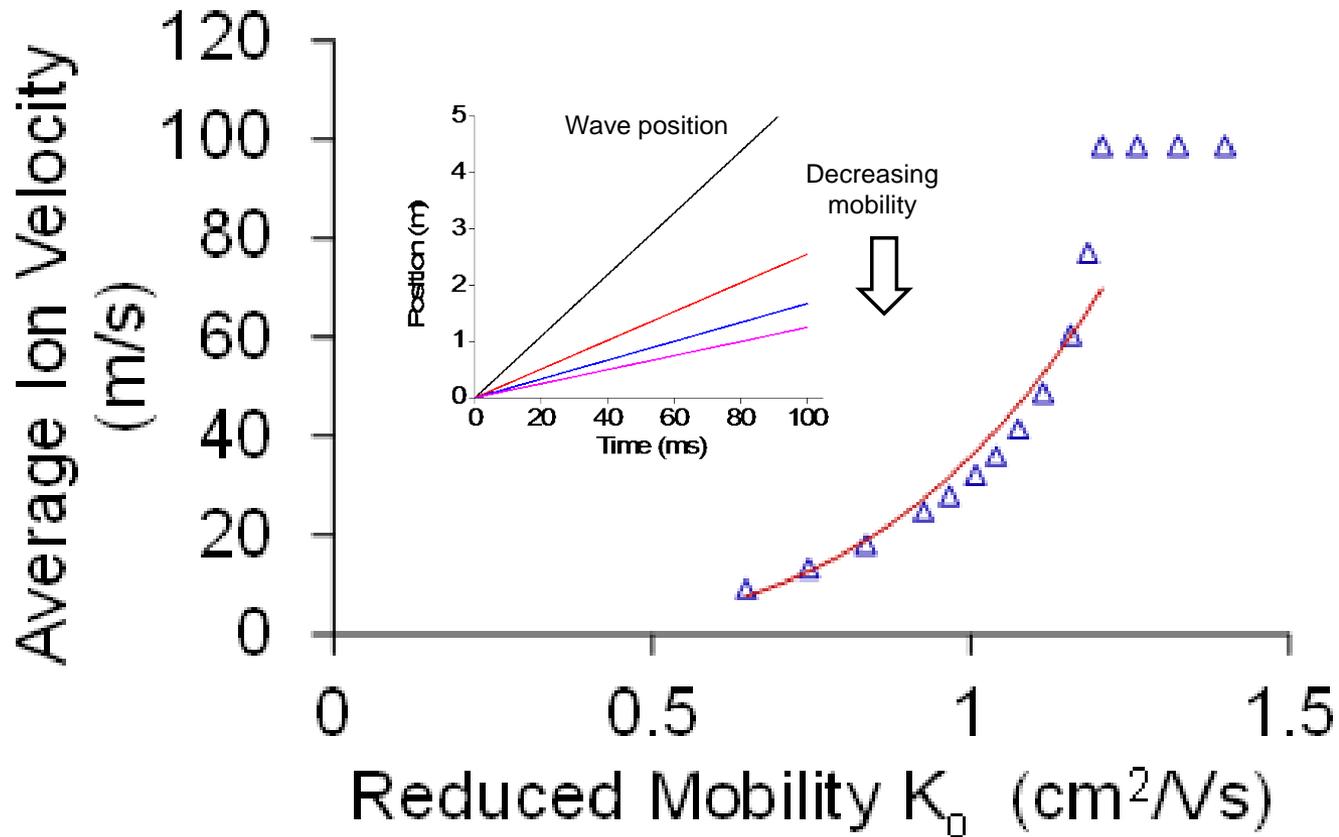
- Pressure ~4 torr to perform IMS separation
- Separation occurs as slower ions execute more number of rollovers into preceding bins

# Average motion of different mobilities



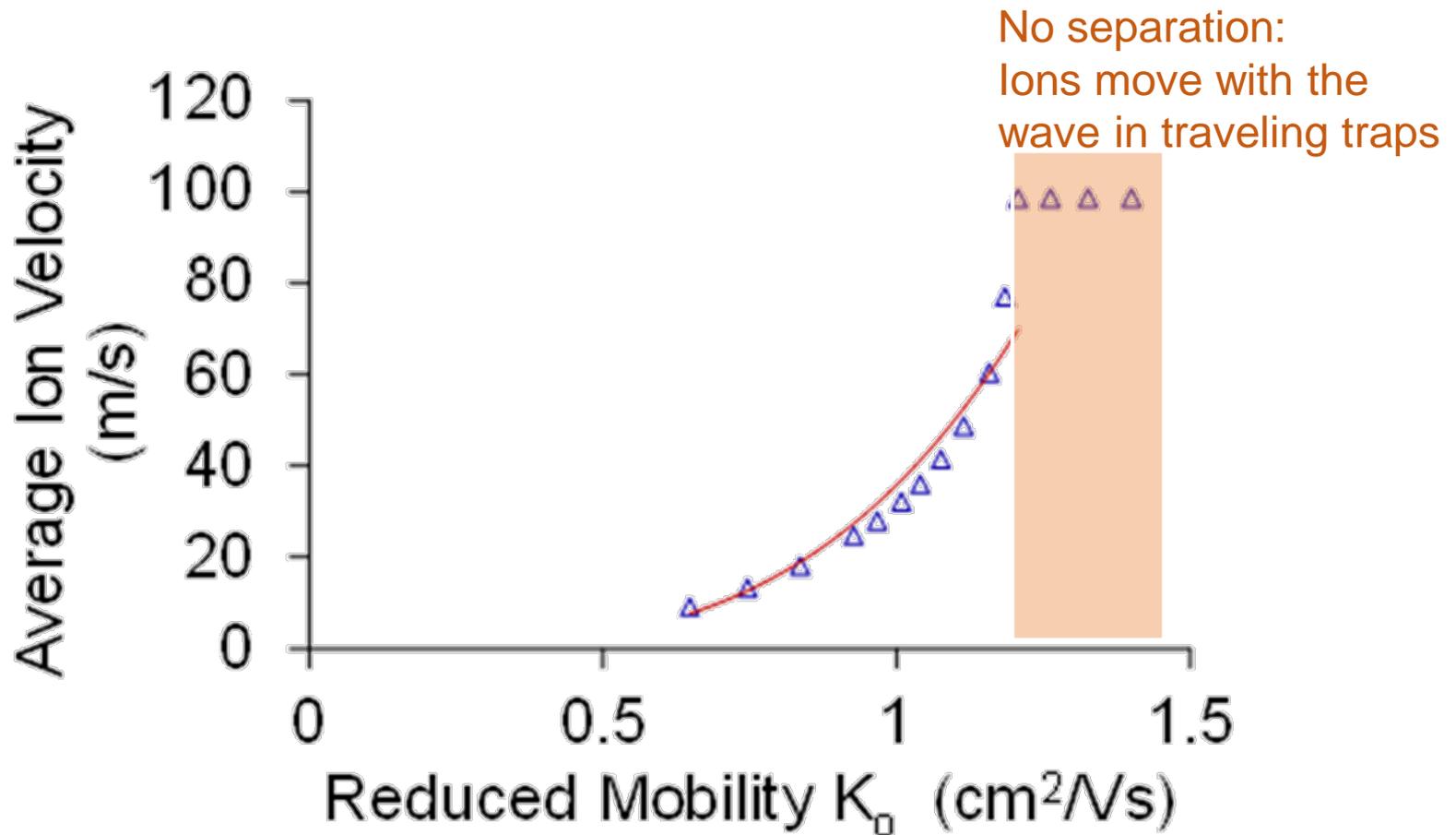
- Over longer flight time the final position of the ions gives average velocity

# Ion velocity in TW-SLIM



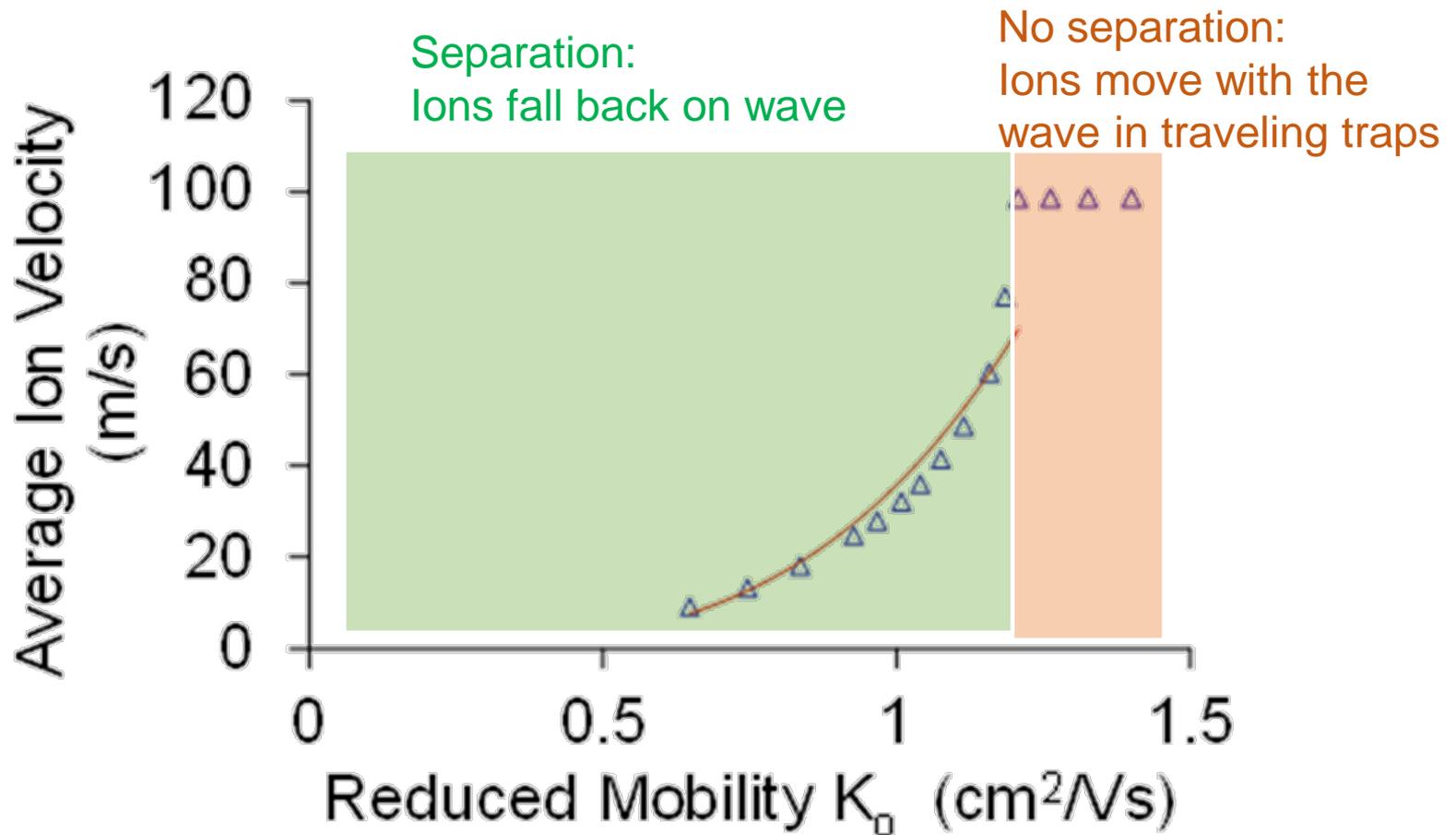
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- The average velocity has non-linear dependence on ion mobility

# Ion velocity in TW-SLIM



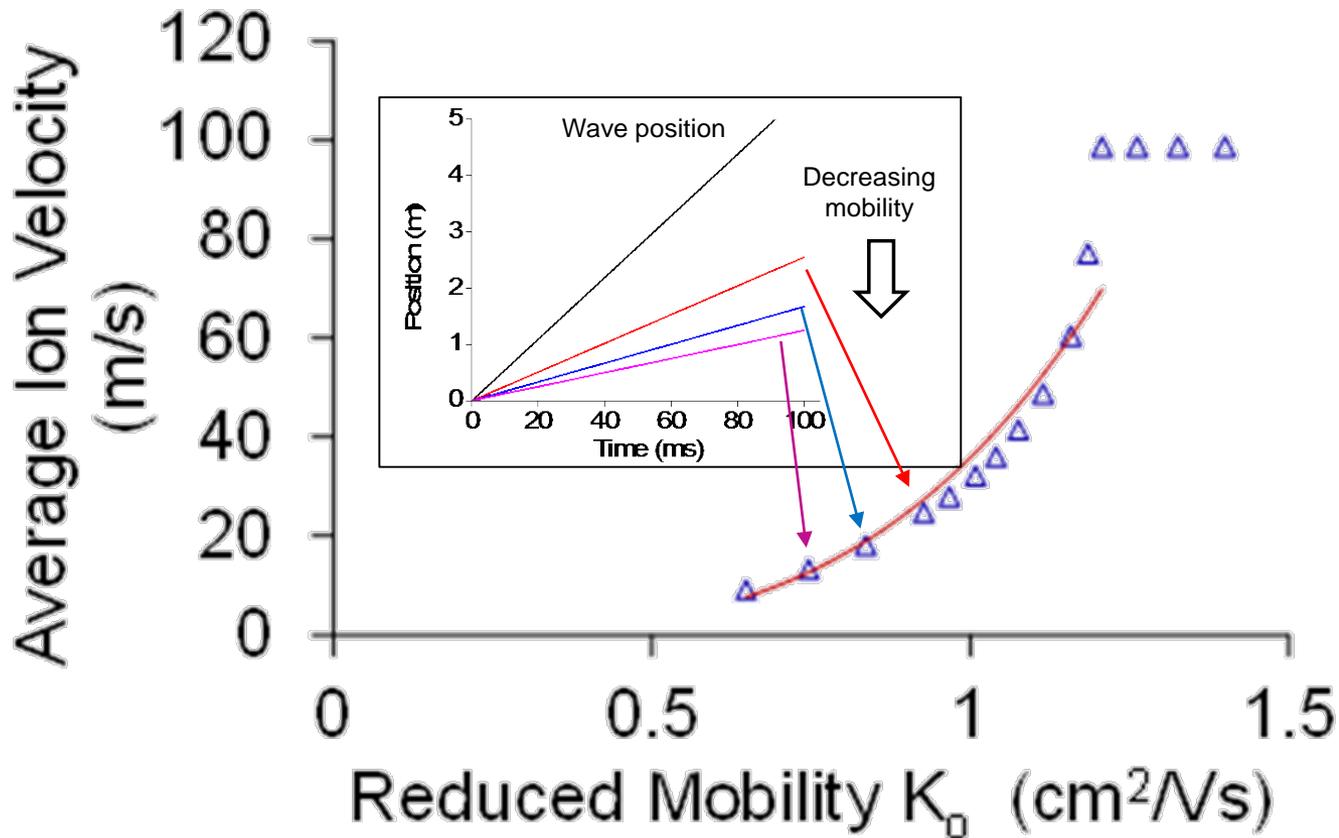
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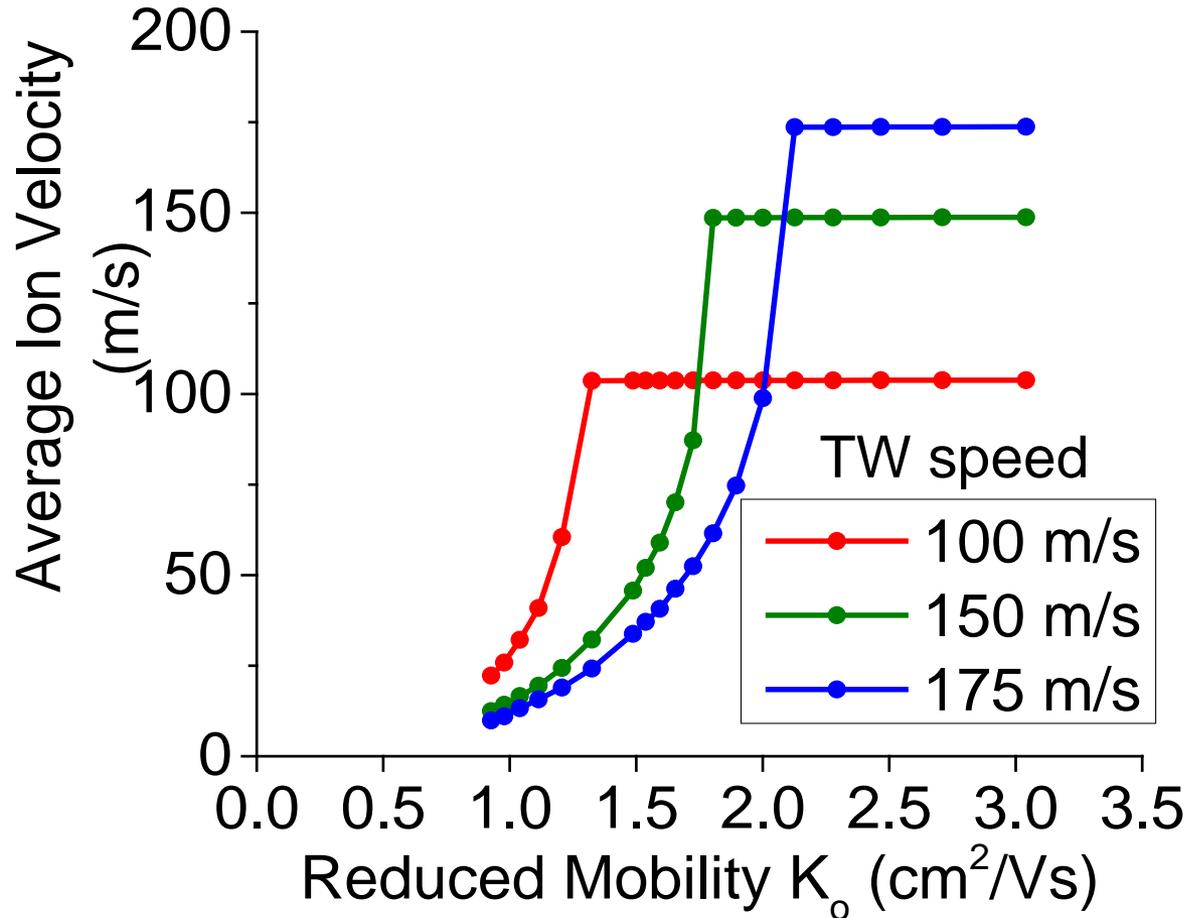
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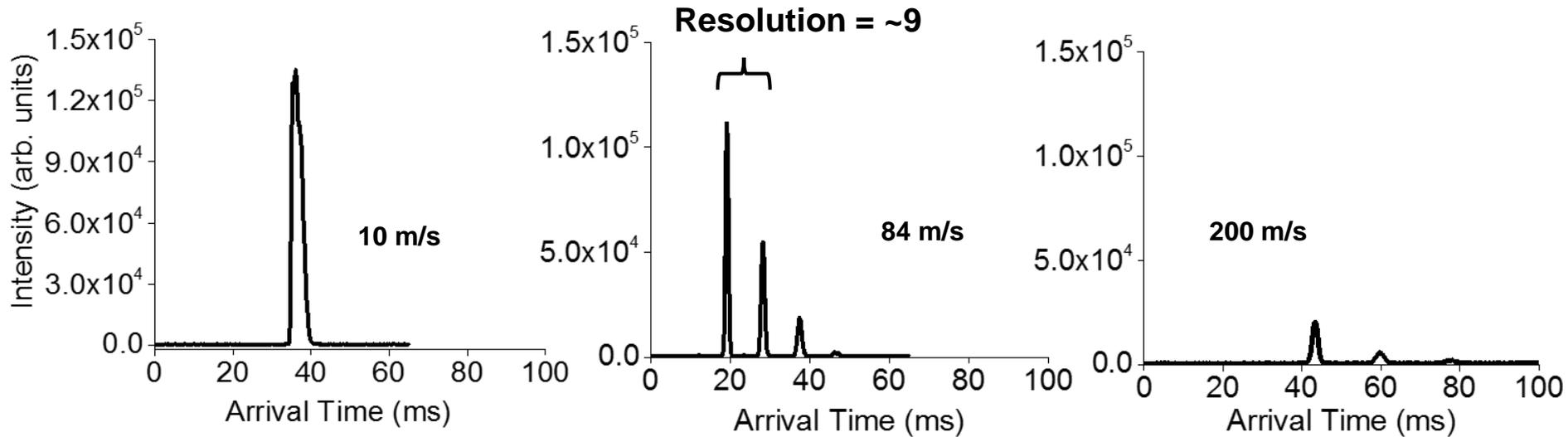
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# Ion velocity in TW-SLIM



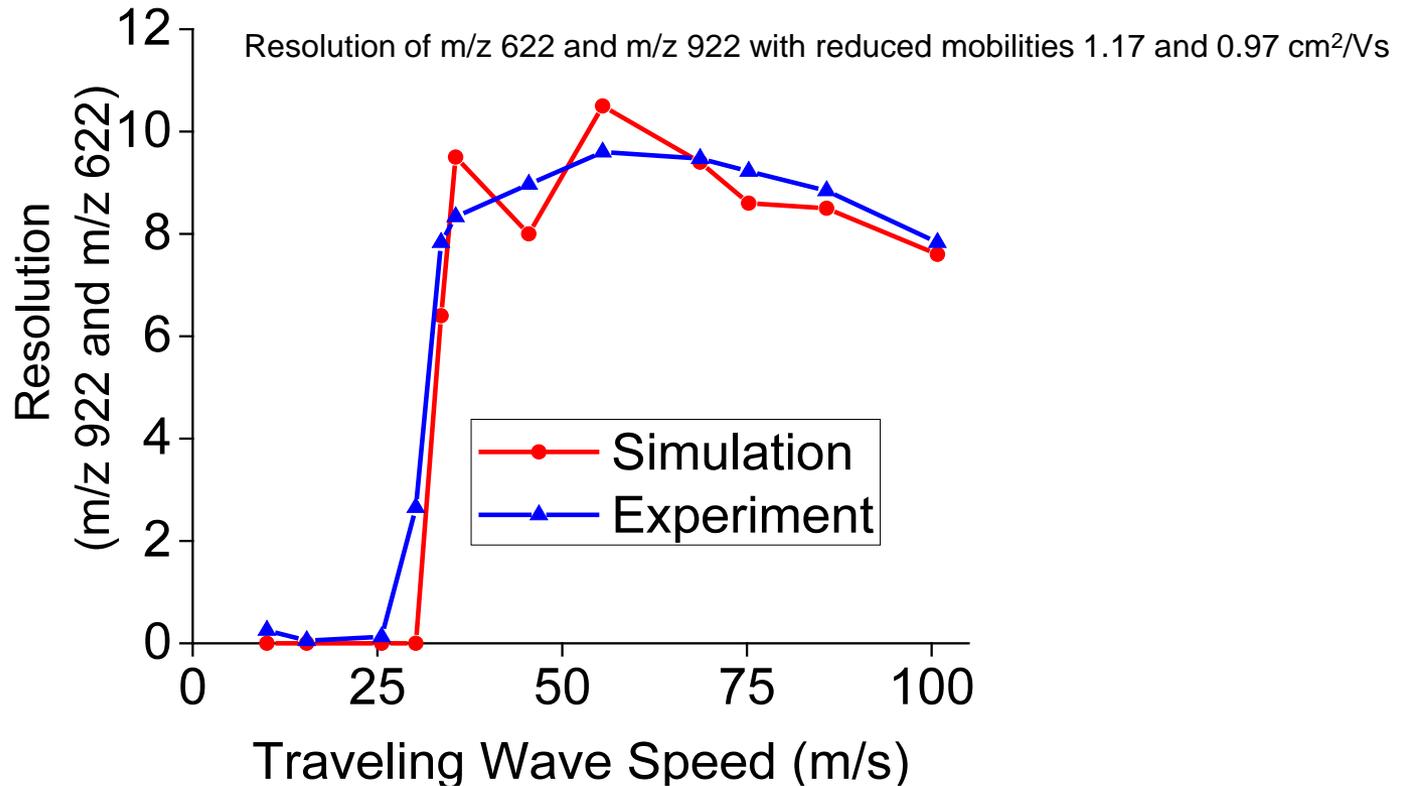
- Over longer flight time the final position of the ions gives average velocity
- The average velocity has non-linear dependence on ion mobility
- Separable mobility range adjusted by changing wave speed

# Mobility based separations



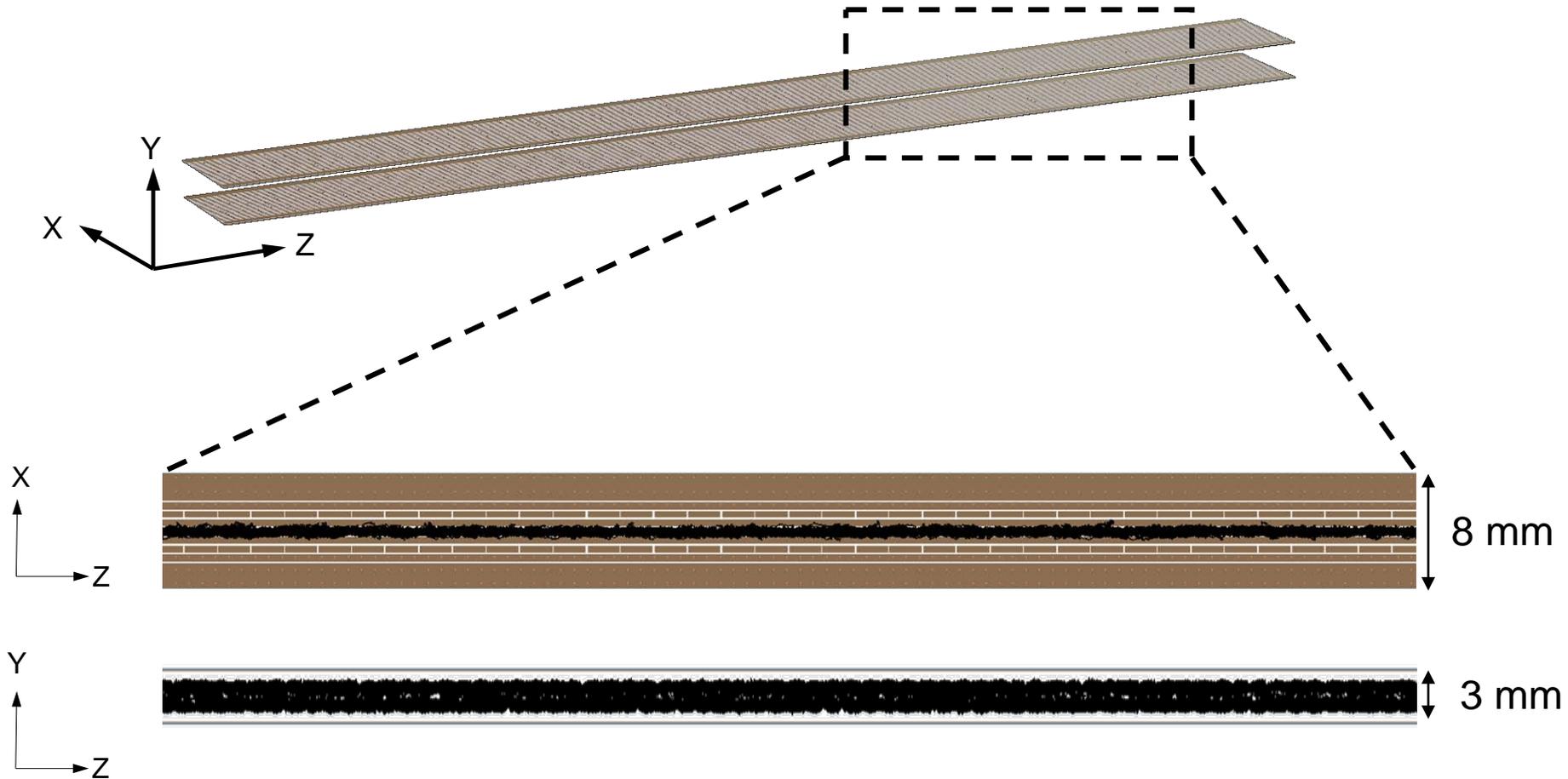
- 30 cm long TW-SLIM IMS with q-TOF MS
- Obtained resolution comparable with that of a 1m long drift tube IMS

# Mobility based separations



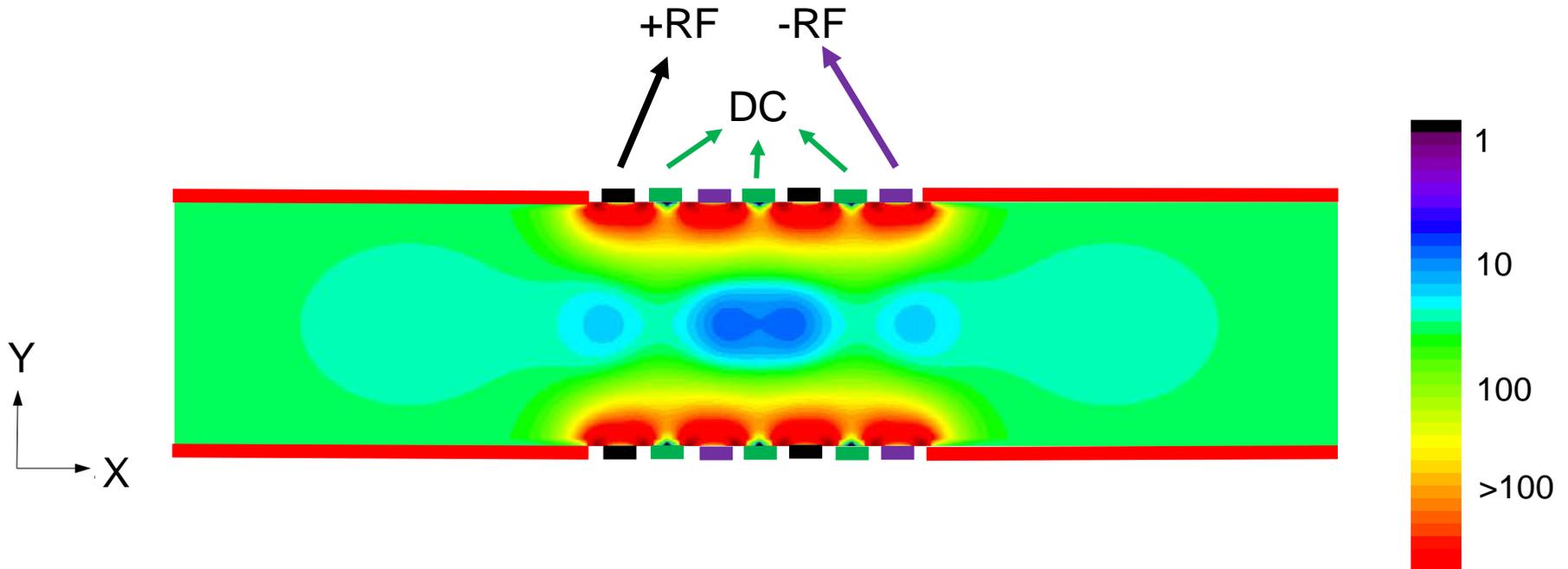
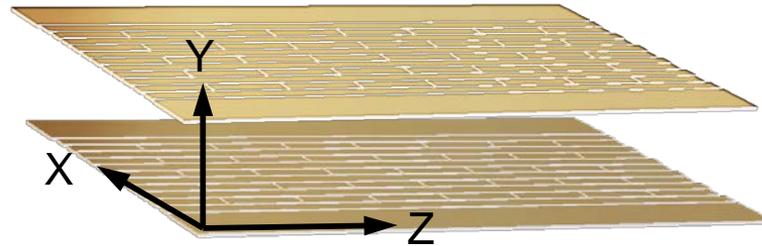
- 30 cm long TW-SLIM IMS with q-TOF MS
- Obtained resolution (~10) comparable with a 1m long drift tube IMS

# Lossless ion transmission feasible



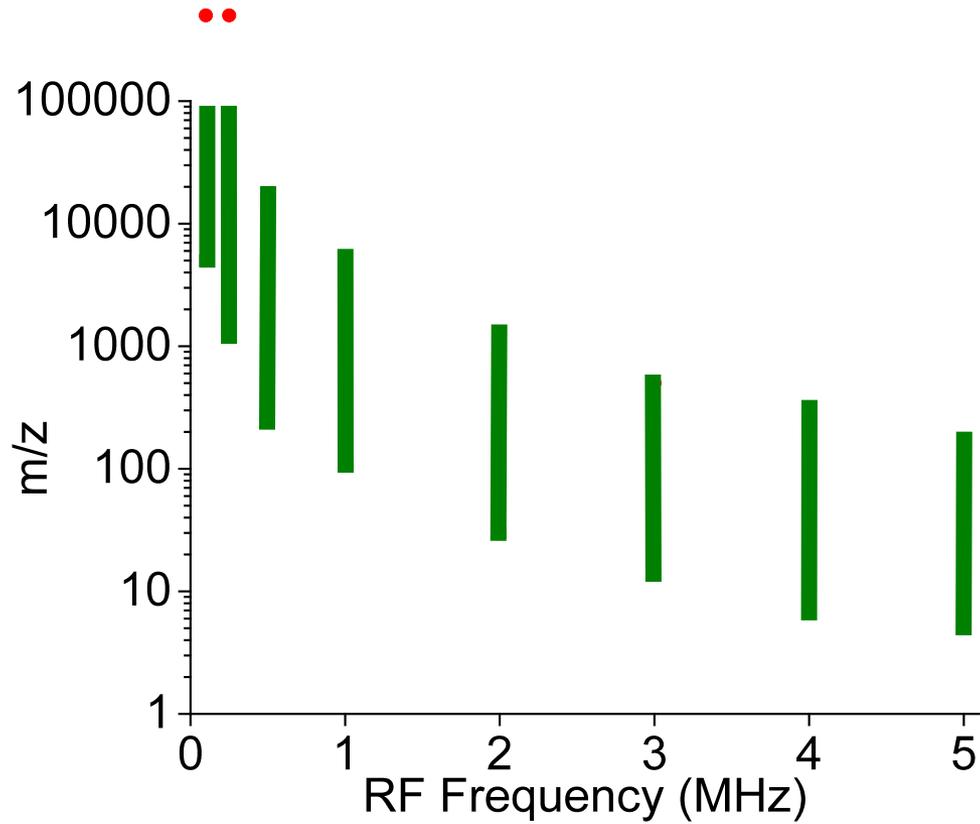
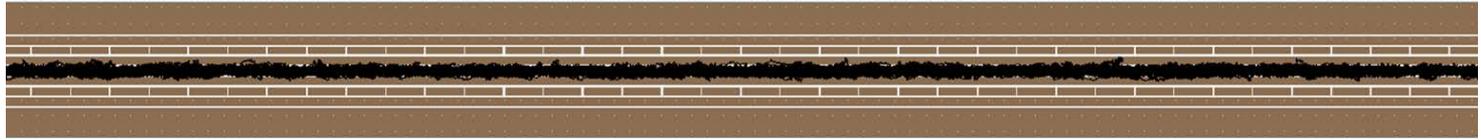
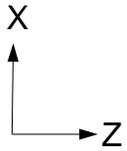
SIMION 8.1 simulation showing lossless ion motion in a 30 cm TW-SLIM

# Ion Confinement in SLIM



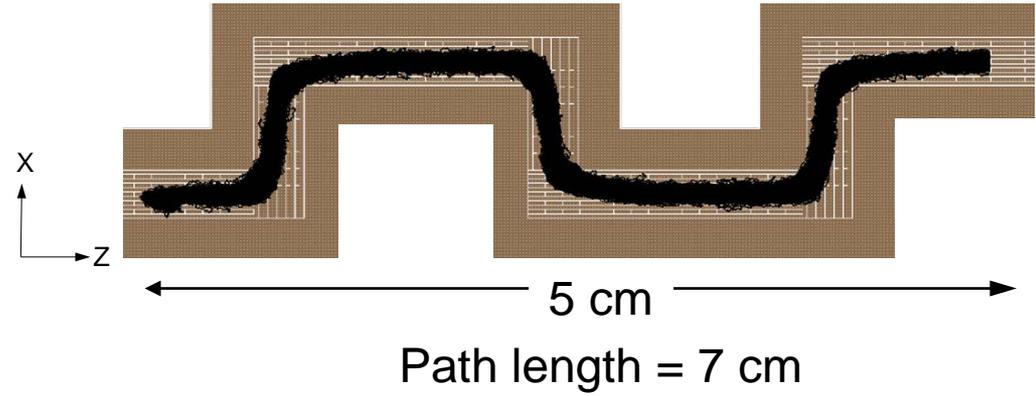
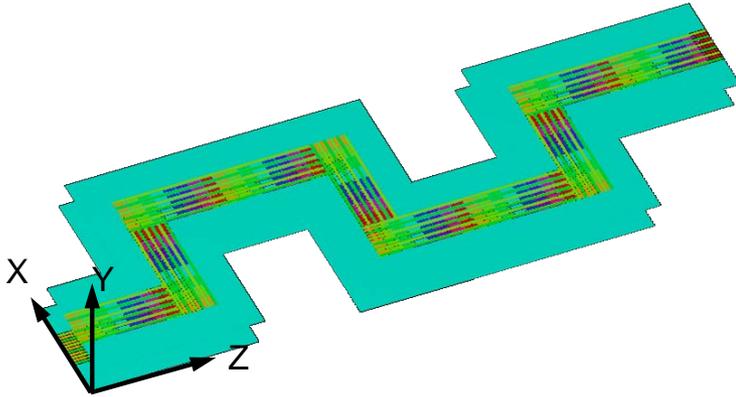
Net potentials that confine ions between the SLIM surfaces

# Mass Range



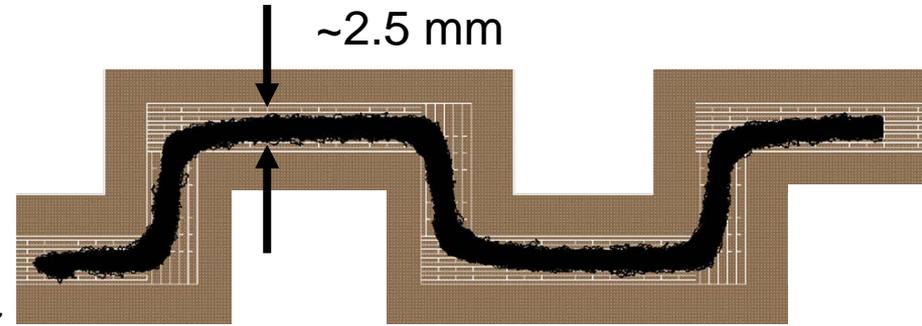
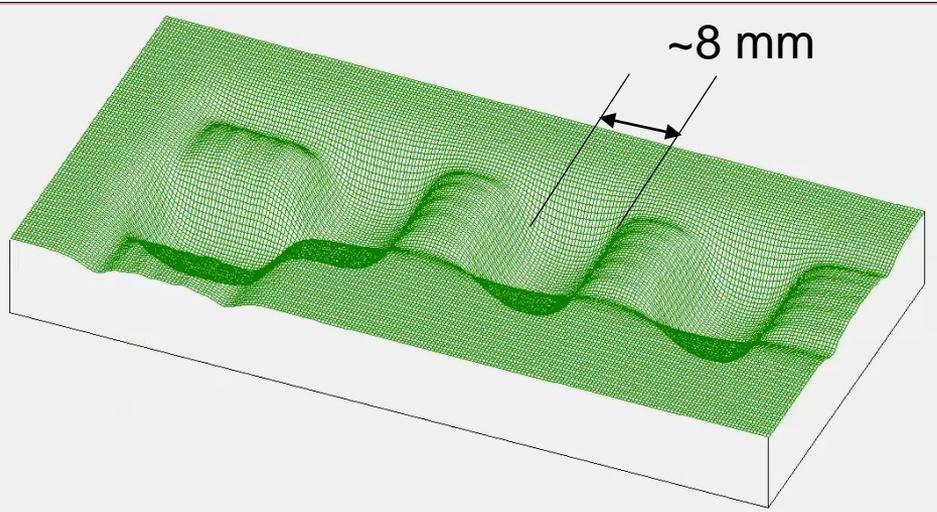
Green bands show mass ranges transmitted losslessly in TW-SLIM

# Making lossless turns in SLIM



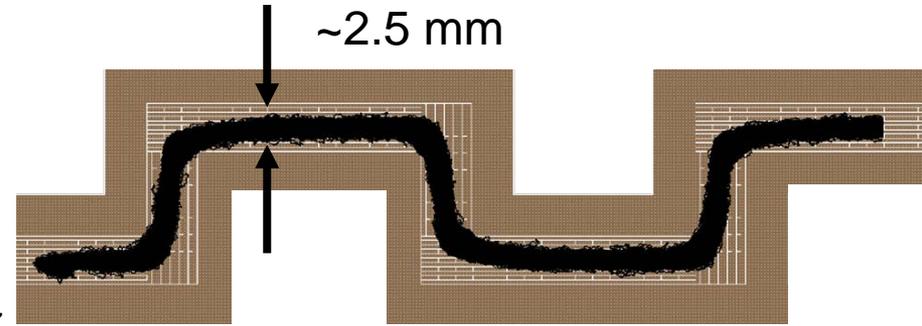
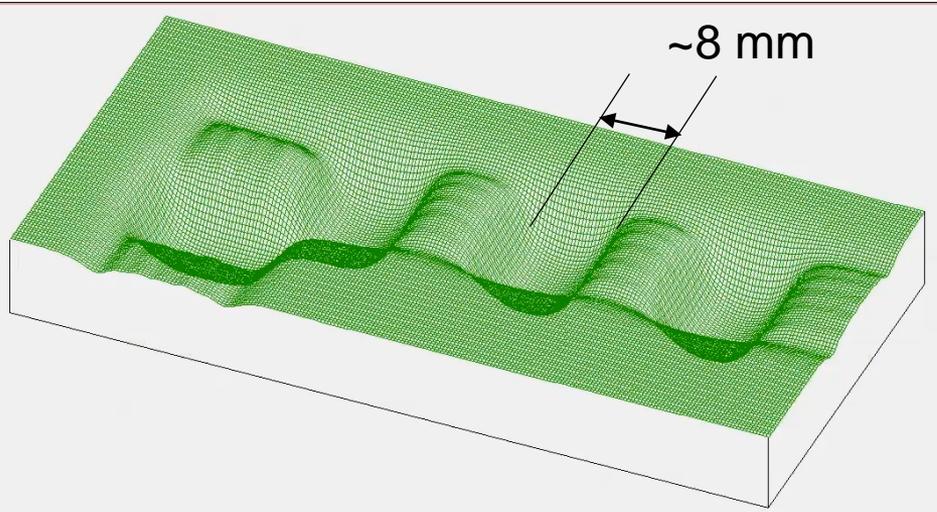
- Serpentine paths allow a compact module to provide extended path length

# Making lossless turns in SLIM



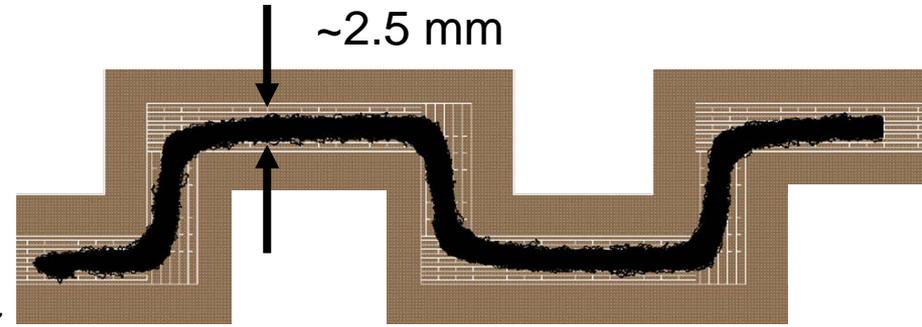
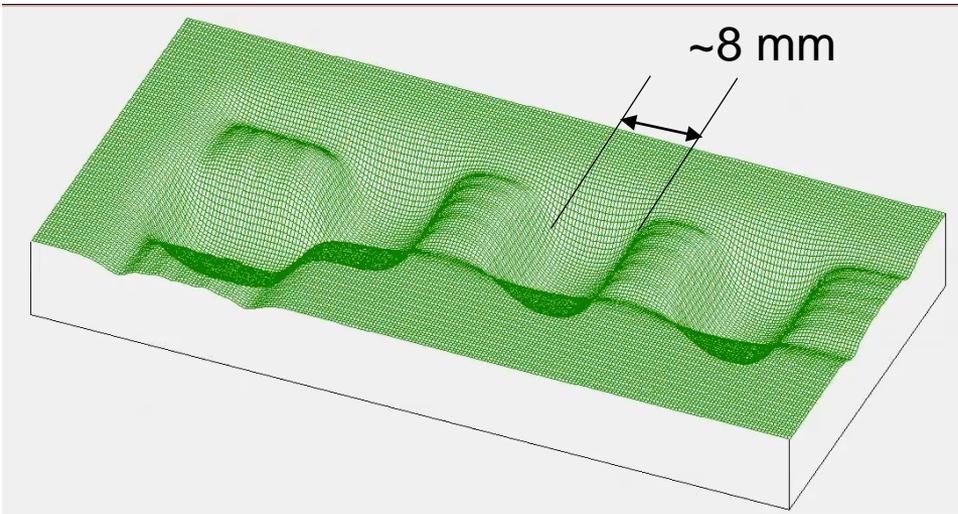
- Serpentine paths allow a compact module to provide extended path length
- Ions from a bin are entrained into the oncoming wave in the orthogonal path

# Making lossless turns in SLIM



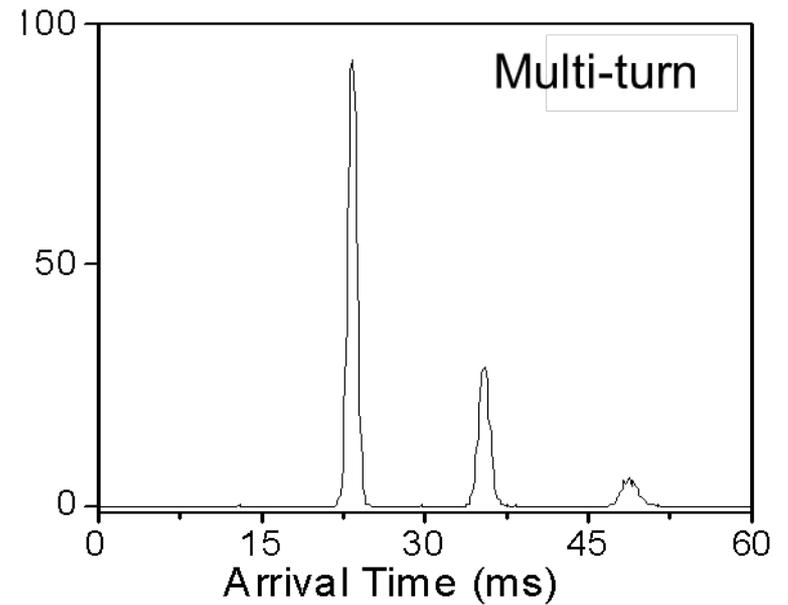
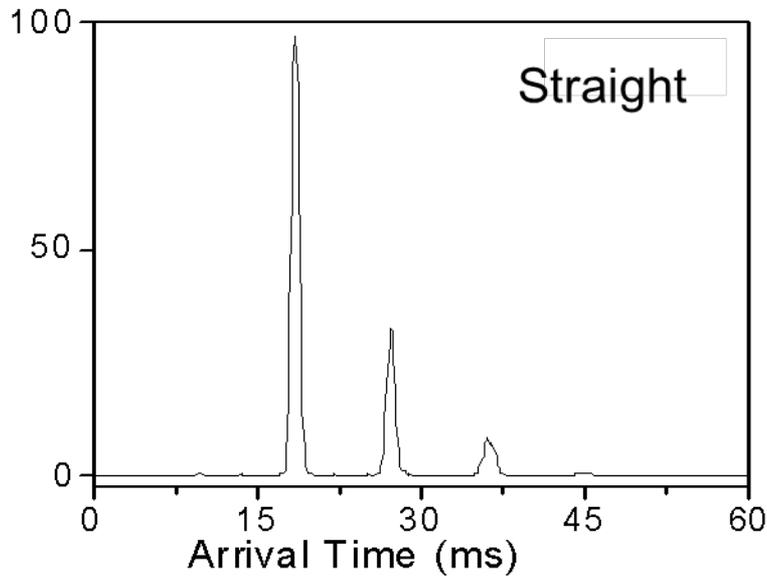
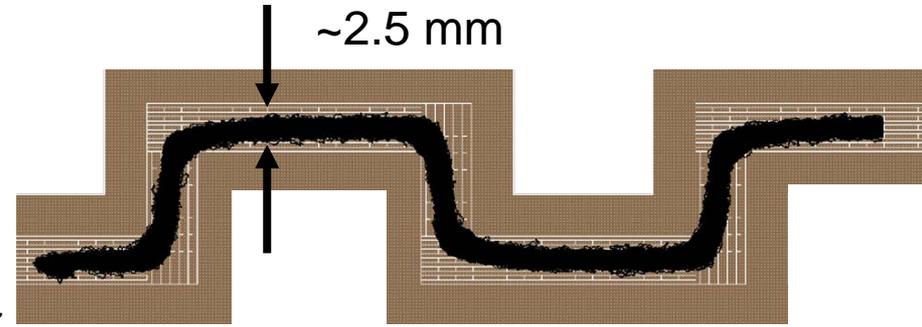
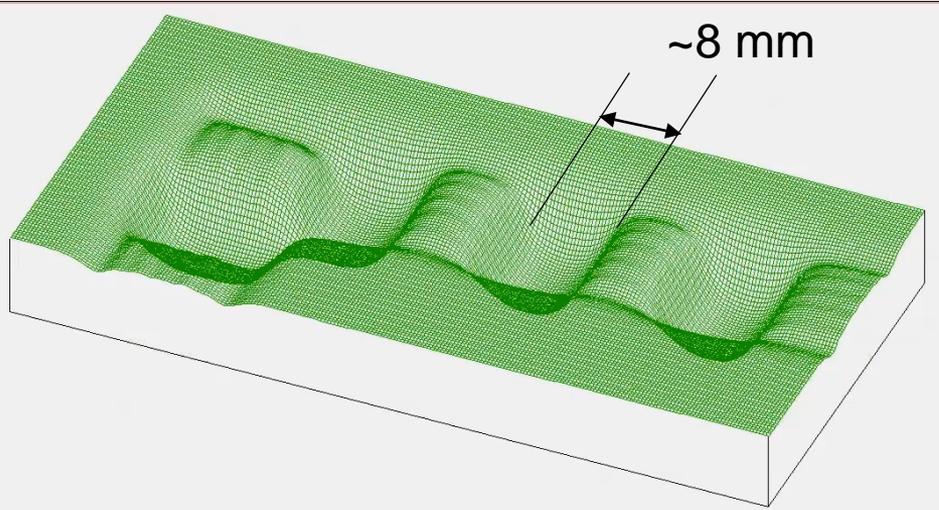
- Serpentine paths allow a compact module to provide extended path length
- Ions from a bin are entrained into the oncoming wave in the orthogonal path
- No “race track” effect

# Making lossless turns in SLIM



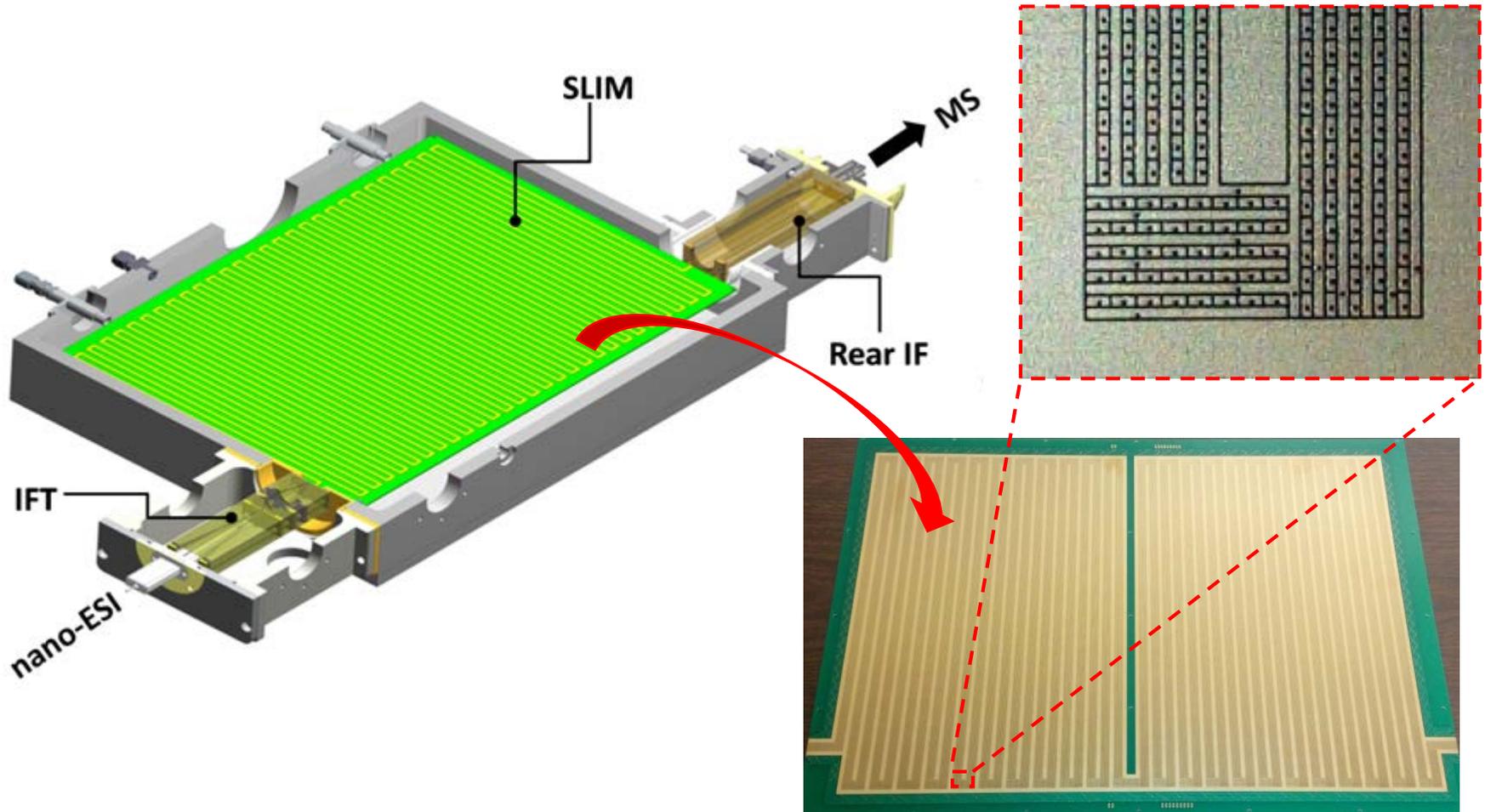
- Serpentine paths allow a compact module to provide extended path length
- Ions from a bin are entrained into the oncoming wave in the orthogonal path
- No “race track” effect
- At turn region, ions can only move forward without rollovers

# Making lossless turns in SLIM



# 13-m path length SLIM IMS-MS

90 turns, 32 cm x 45 cm surface



# 13-m path length SLIM IMS-MS

Fast Separations

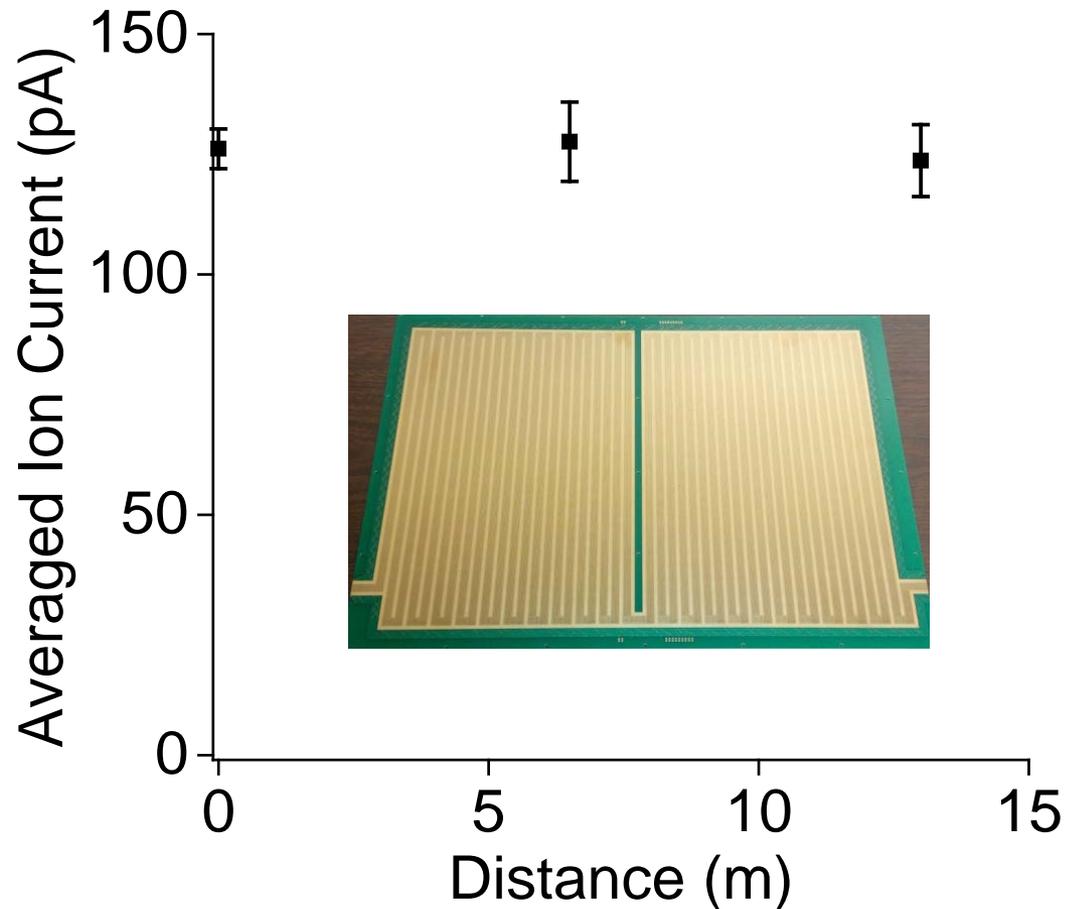


High Resolution



High Sensitivity

Lossless



# 13-m path length SLIM IMS-MS

Fast Separations



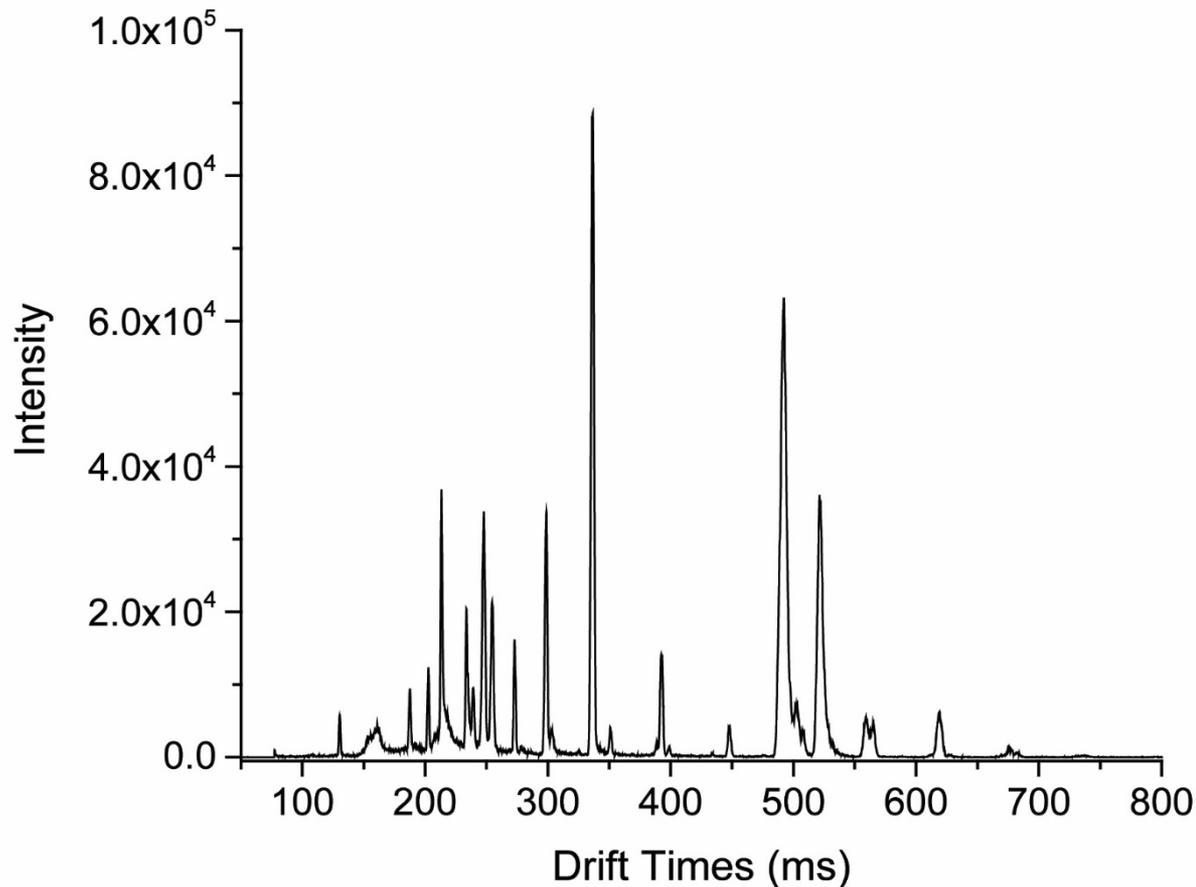
High Resolution



High Sensitivity

<1s separations

Lossless



# 13-m path length SLIM IMS-MS

Fast Separations



High Resolution

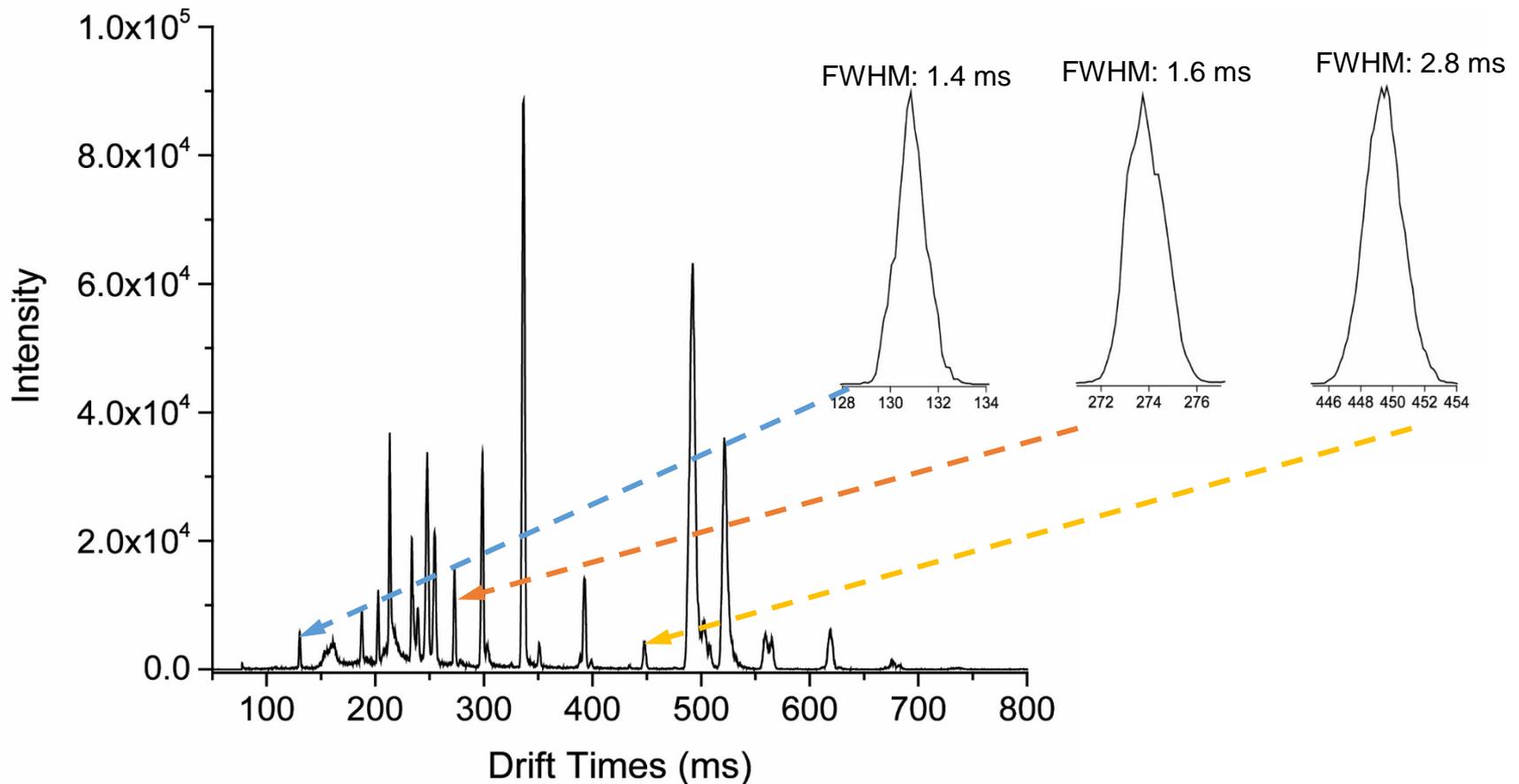


High Sensitivity

<1s separations

peak capacity  
~ 300

Lossless



# Better separations coming.....

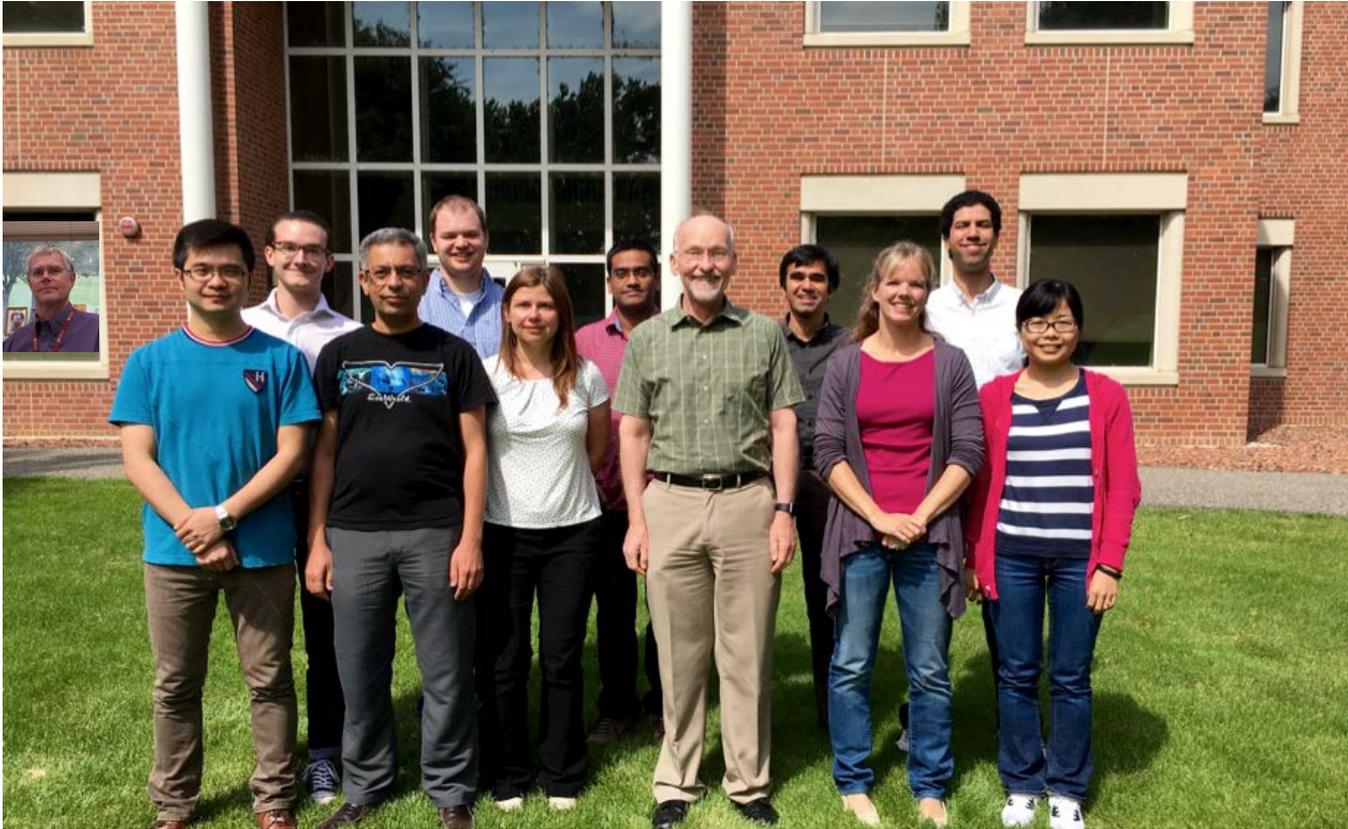
- Build even more extended separations to dramatically improve peak capacities
- Use SLIM elevator concept to build multi-turn, multi-level boards
- Other novel separations such as ion mobility filters
- SLIM designs accommodating large ion currents

# Summary

- TW-IMS enables separations using a fixed moving voltage profile
- SLIM enable lossless ion transport
- Fundamental understanding of ion velocities in TW-SLIM gives insights into separation process and to build complex designs
- Ability perform extended ion manipulations allows extended path lengths (13 m initially demonstrated)

# Acknowledgements

PNNL SLIM Team



## \$upport

National Institute of General Medical Sciences  
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DOE Office of Biological and Environmental Research