NVMS – BSMS 2024
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Sliding windows in ion mobility (SWIM): a new approach to increase the separation power in trapped ion mobility-mass spectrometry hyphenated with chromatography

MASS SPECTROMETRY LABORATORY

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PhD student

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Introduction

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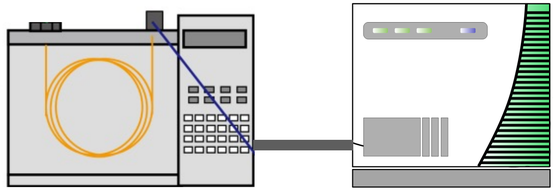
Hugo B. Muller et. al, “Sliding windows in ion mobility (SWIM): a new approach to increase the separation power in trapped ion mobility-mass spectrometry hyphenated with chromatography”

POPs analysis in food

Traditional approach



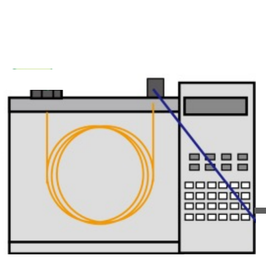
GC

Separates neutrals according to **boiling point**

MS

Separates ions according to **m/z ratio**

Our approach



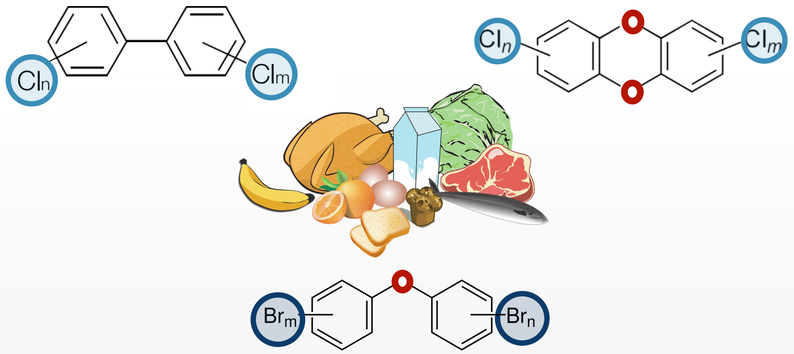
GC

Boiling point

Ion Mobility-MS

Separates ions according to **ion mobility coefficient K**

m/z ratio



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Ion mobility

→ Origin: end of the 19th century
→ First commercial IM-MS instruments: mid-2000s
→ Exponential growth in the last decade

Drift speed

$$v_d = KE$$

Ion mobility coefficient

Fundamental low-field mobility equation

$$K = \frac{3}{16}\sqrt{\frac{2\pi}{\mu k_b T}}\frac{ze}{N\Omega}$$

Charge

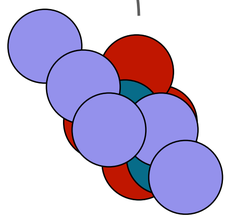
Mass

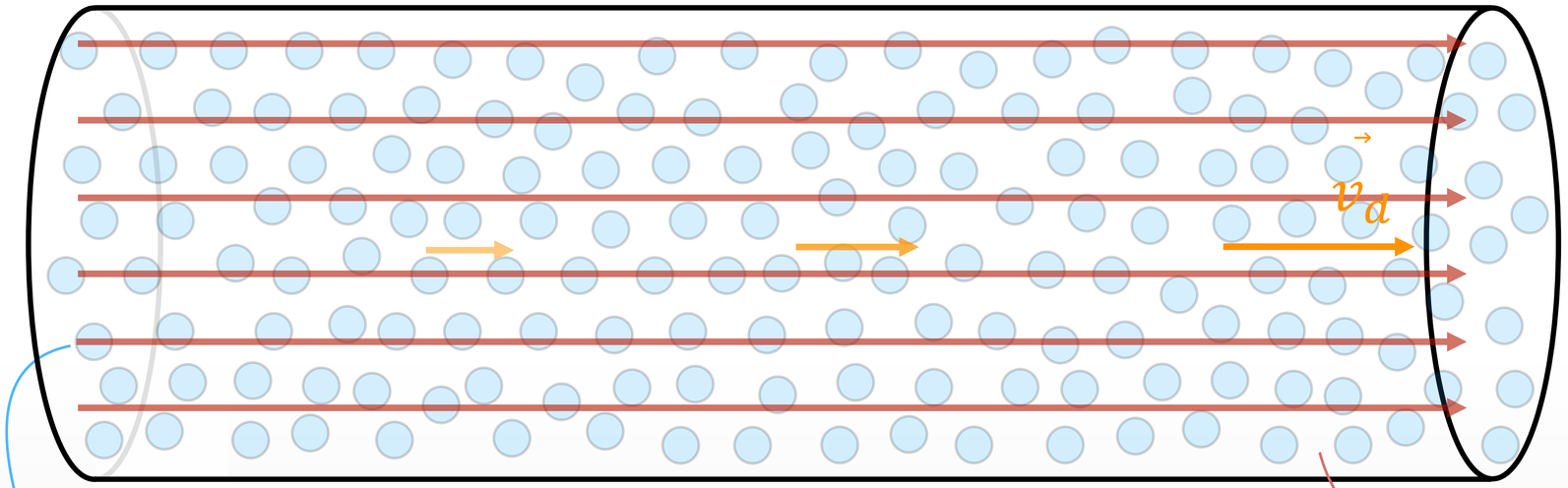
Collision **C**ross **S**ection (**CCS**)

Size & shape

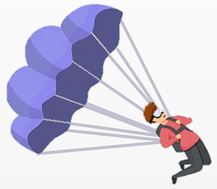
Ion-gas interaction potential

Mixture of ions



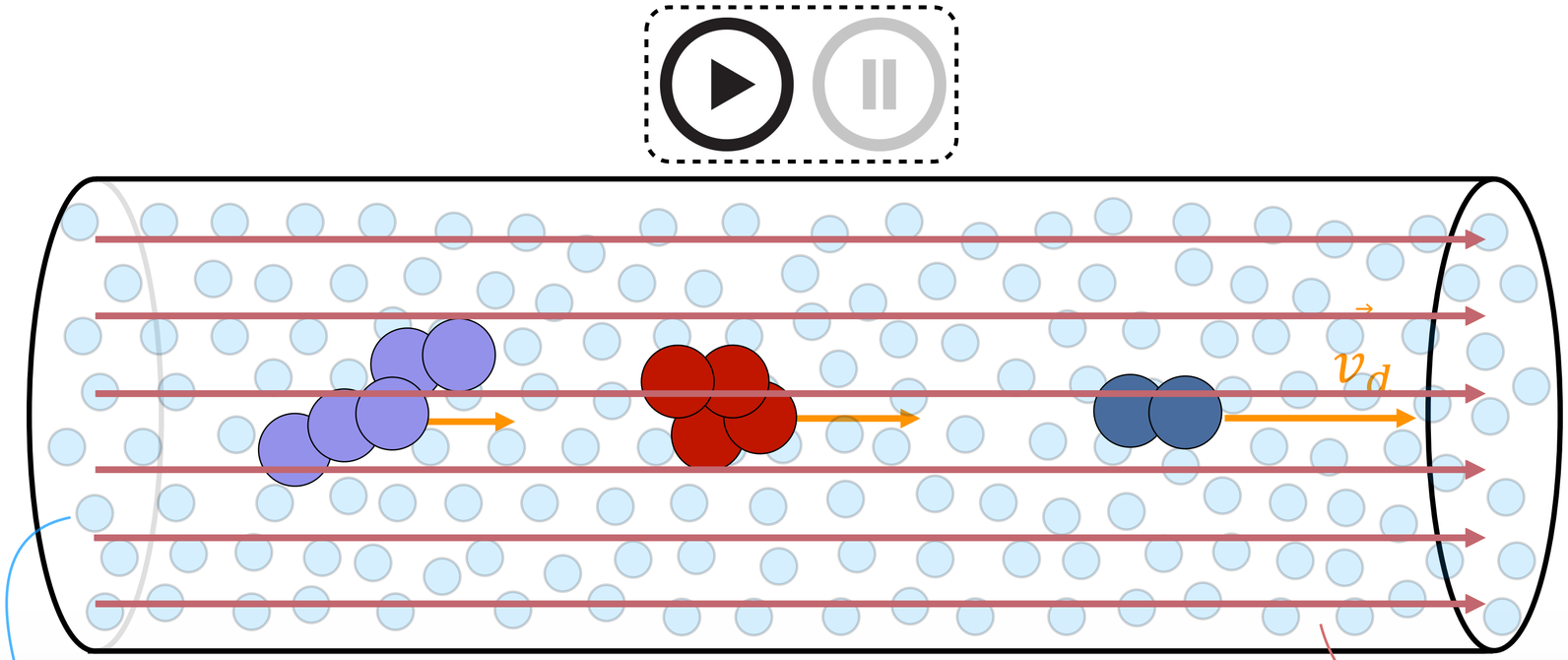


Drift gas (N_2)

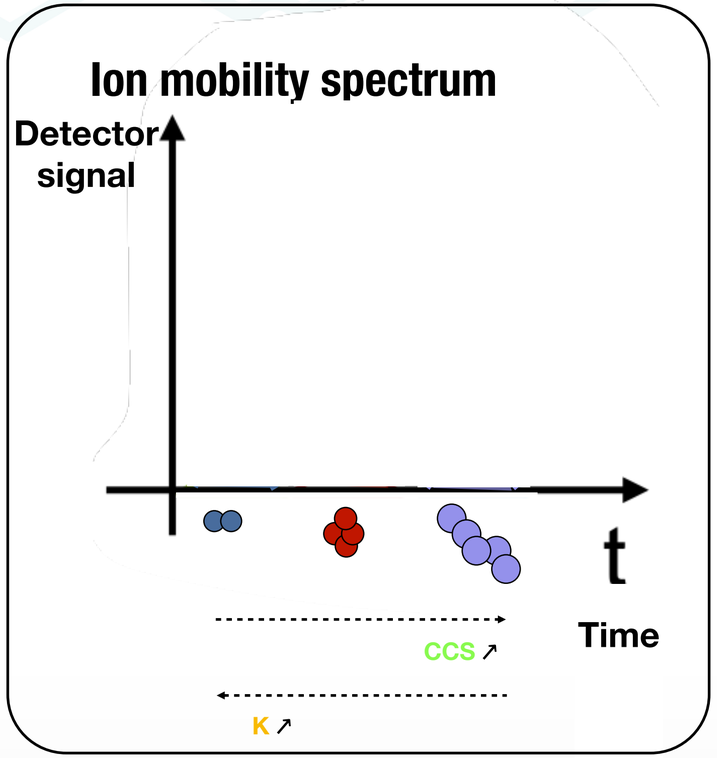


Electric field $\vec{E}$

Ion mobility



$\vec{v}_d$



Drift gas (N_2)

Electric field $\vec{E}$

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Ion mobility

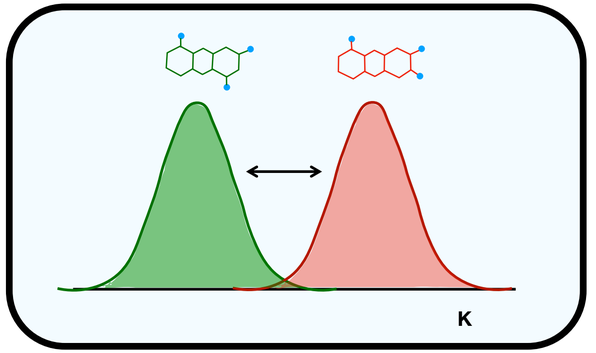
Technologies

- DTIMS
- TWIMS
- FAIMS/DMS
- TIMS

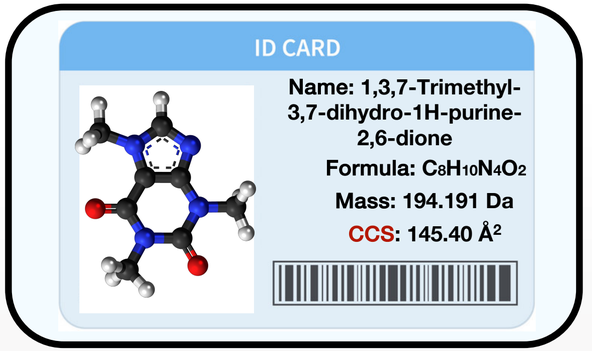
Ion mobility - mass spectrometry (IM-MS)

Advantages

- **Selectivity**
  - Isomers & Isobars
  - Background removal



- **Identification** — CCS



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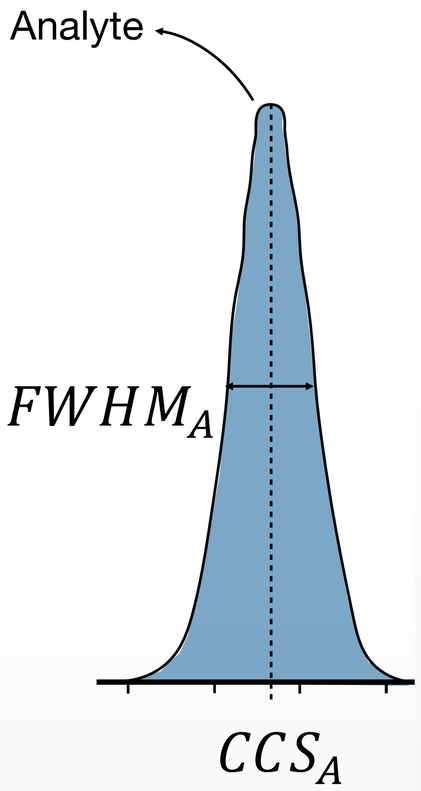
Resolving power

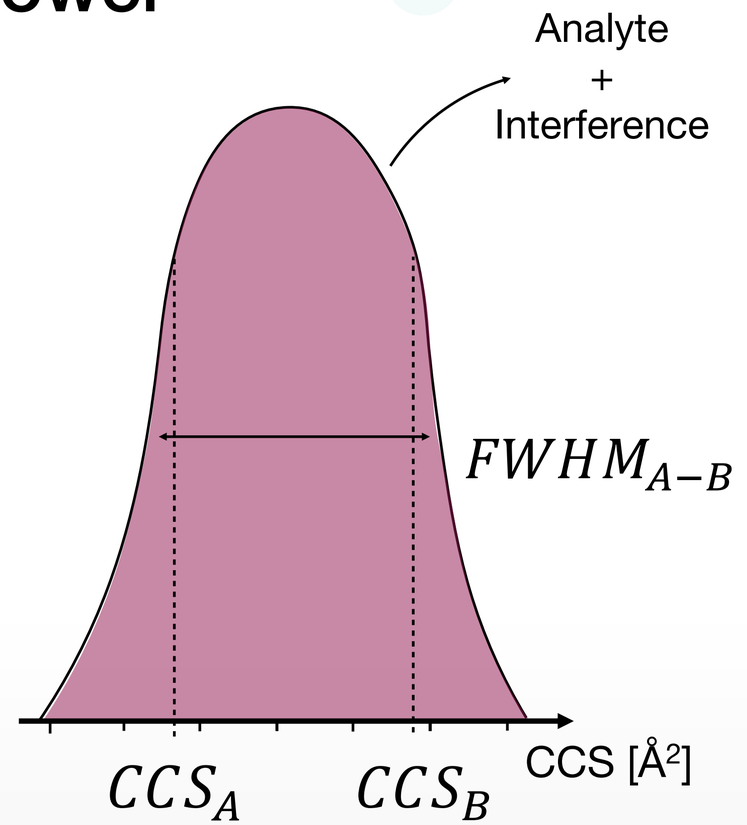
High resolving power



Resolving power

$$R_p = \frac{CCS_X}{FWHM_X}$$

Low resolving power



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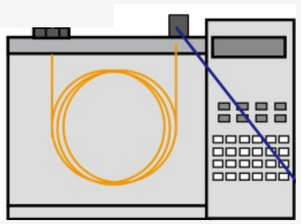
Rp in TIMS

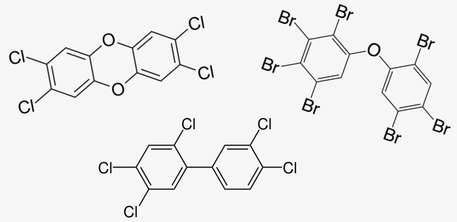
GC coupling



⇒ Fast IM separations

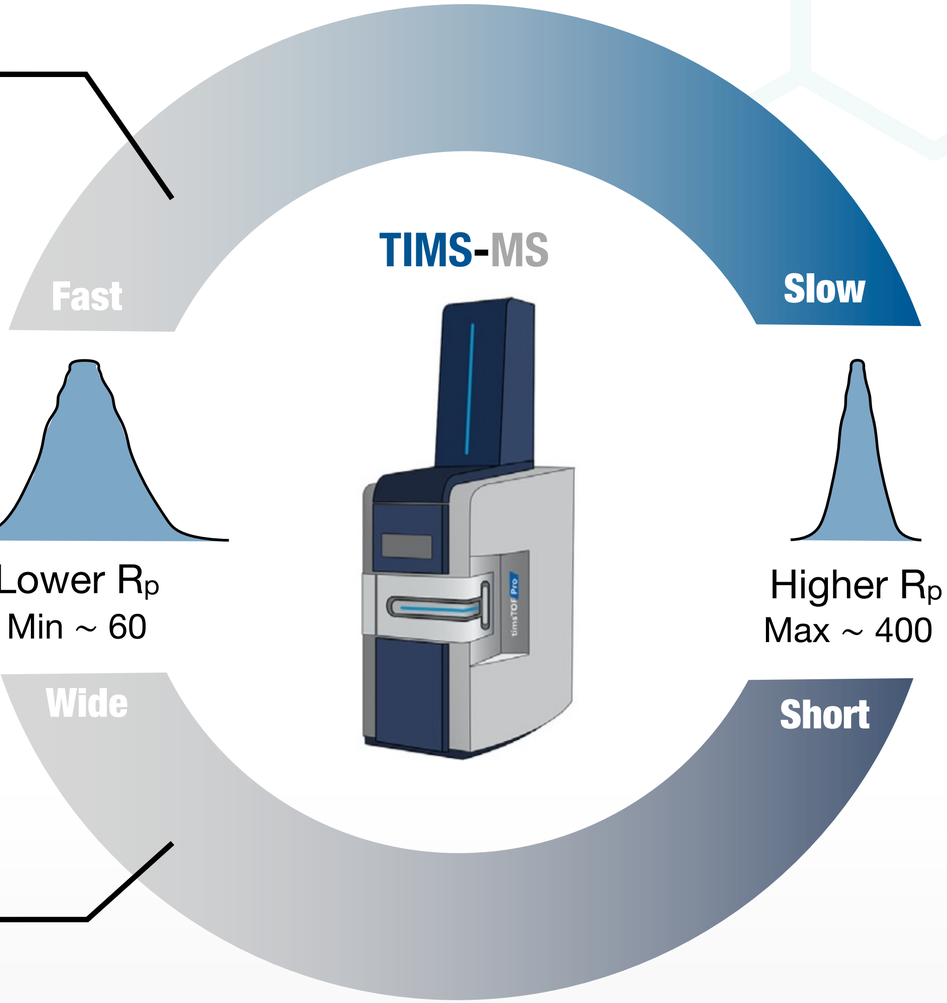
Limited R_p

Diversity of POPs



⇒ Wide IM range

Analysis time



5th joint NVMS/BSMS conference on Mass Spectrometry (Rolduc 2024)
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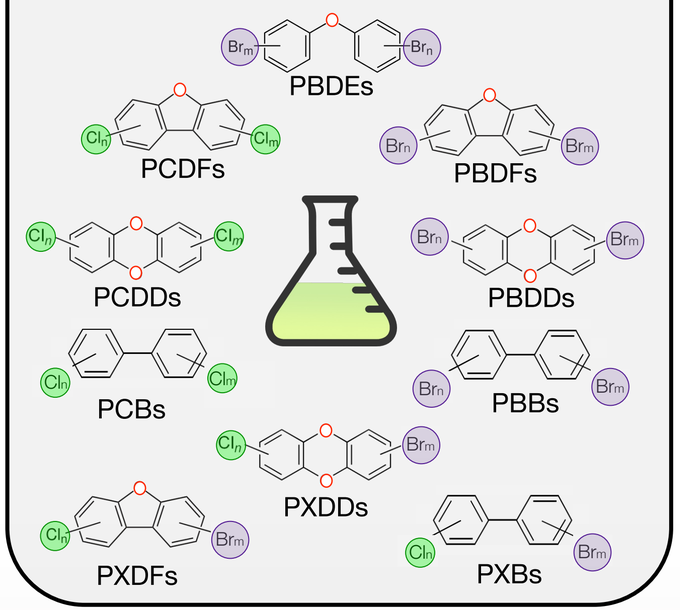
Rp in TIMS

Mixture of 174 POP standards

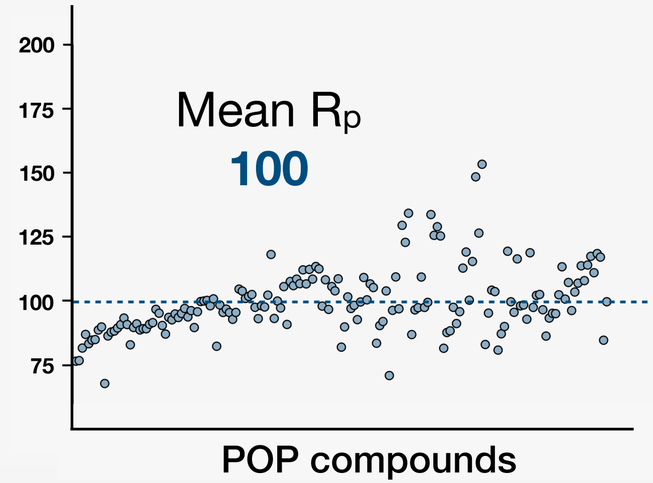


GC-TIMS-MS analysis

Analysis time:
350 ms

IM range:
1.00 - 1.67 K_0

Resolving power



Can we still improve the **resolving power**?!

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SWIM

Sliding Windows in Ion Mobility

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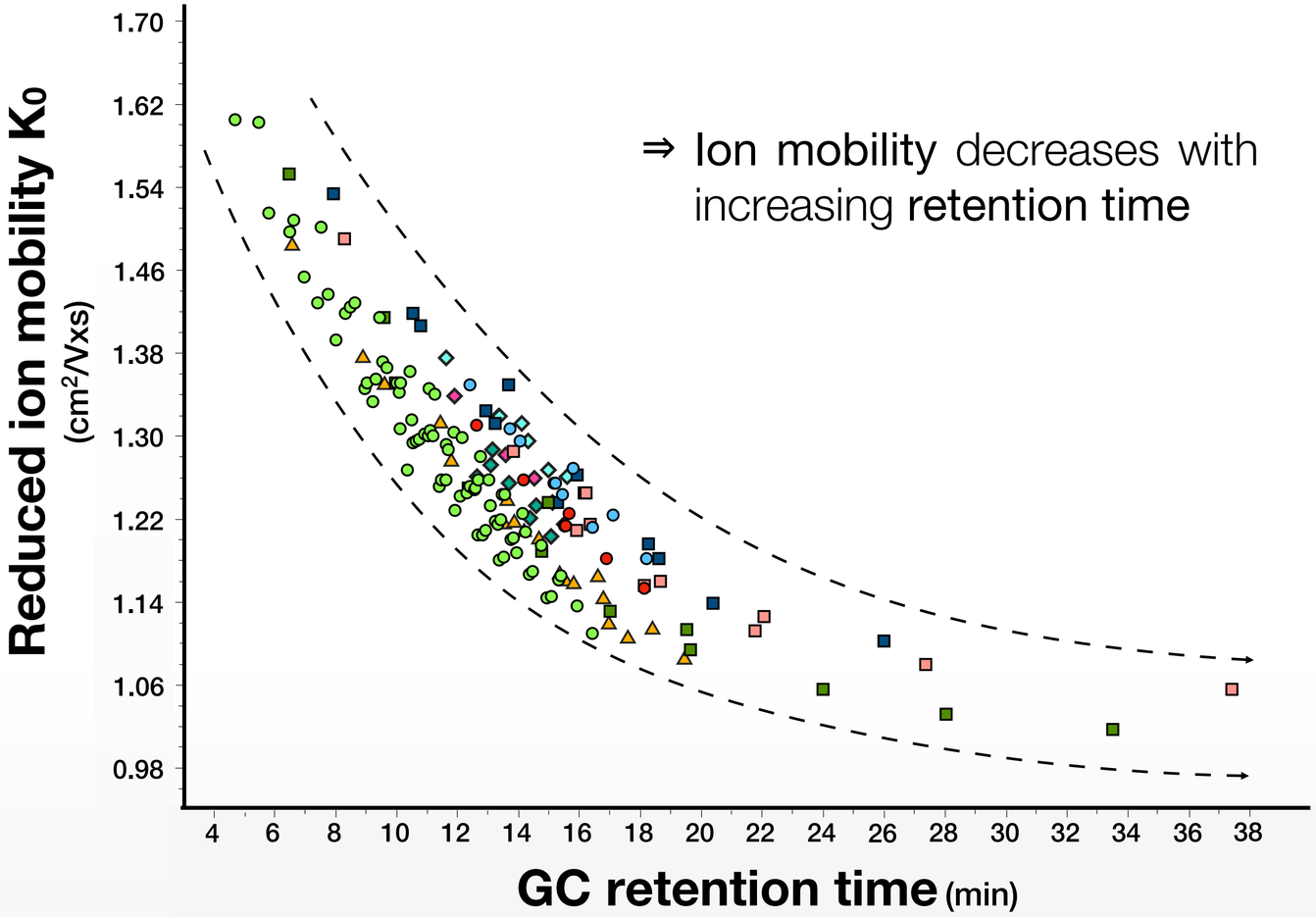
RT vs K correlation



⇒ Ion mobility decreases with increasing **retention time**

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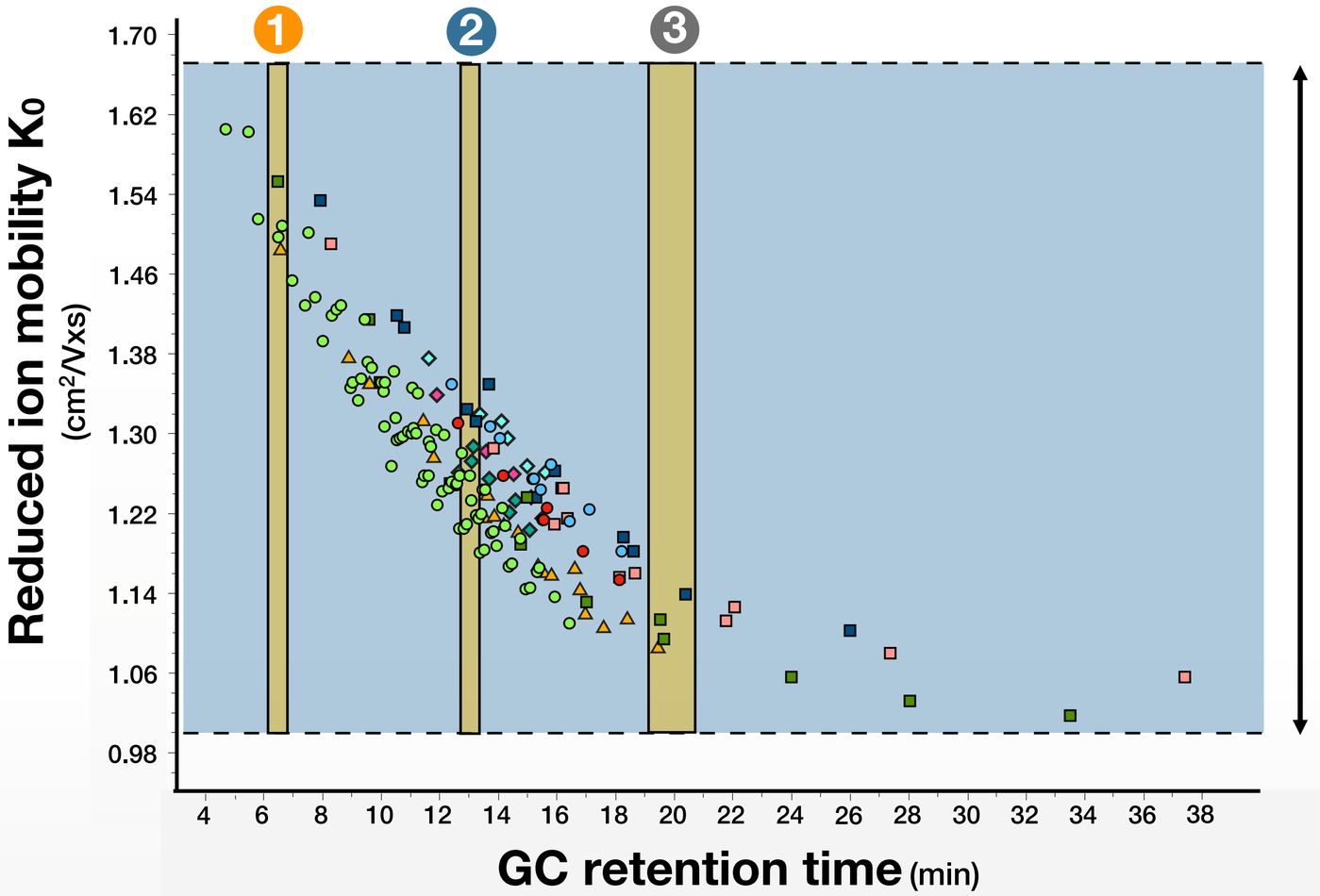
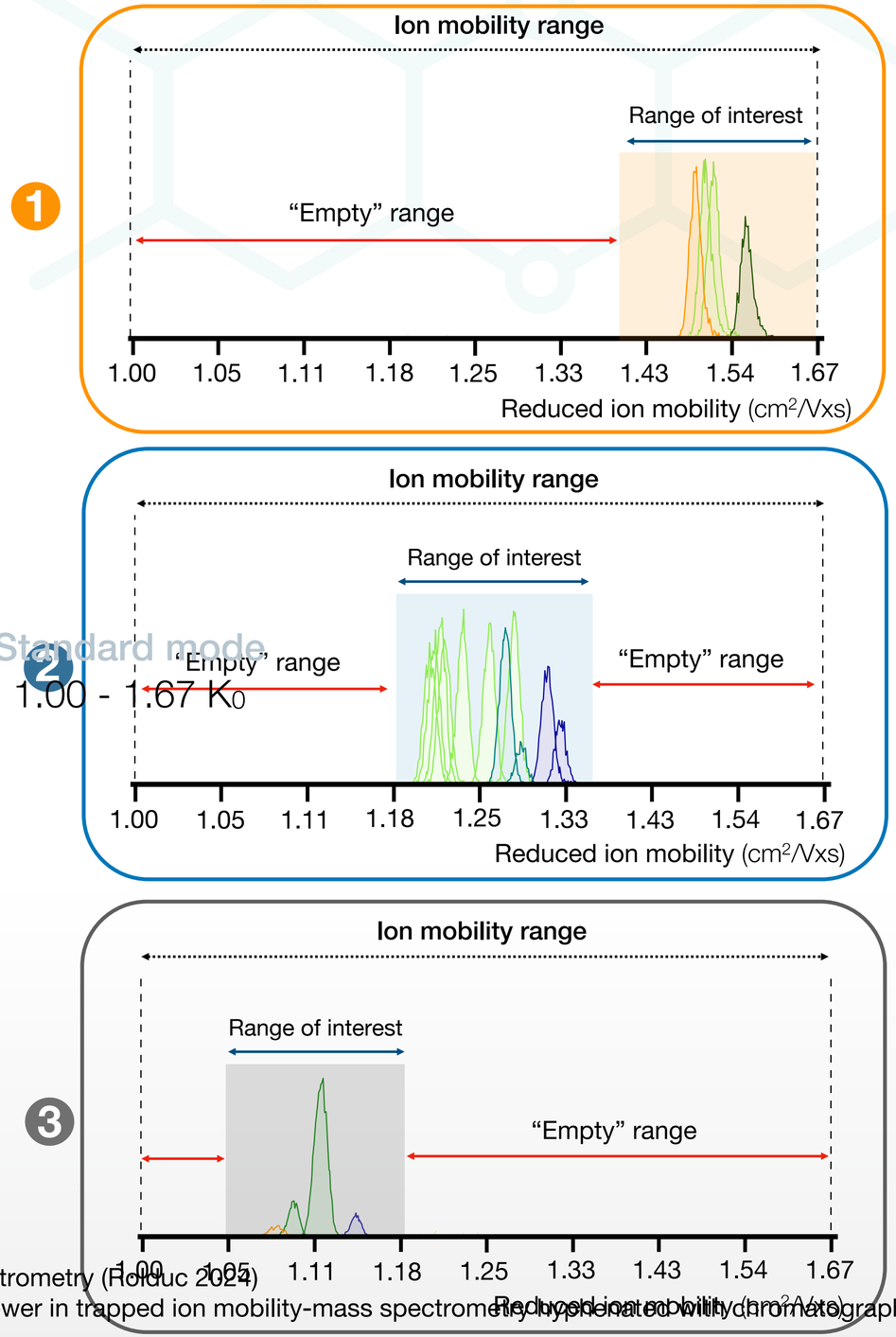
Standard mode





Standard mode
1.00 - 1.67 K_0

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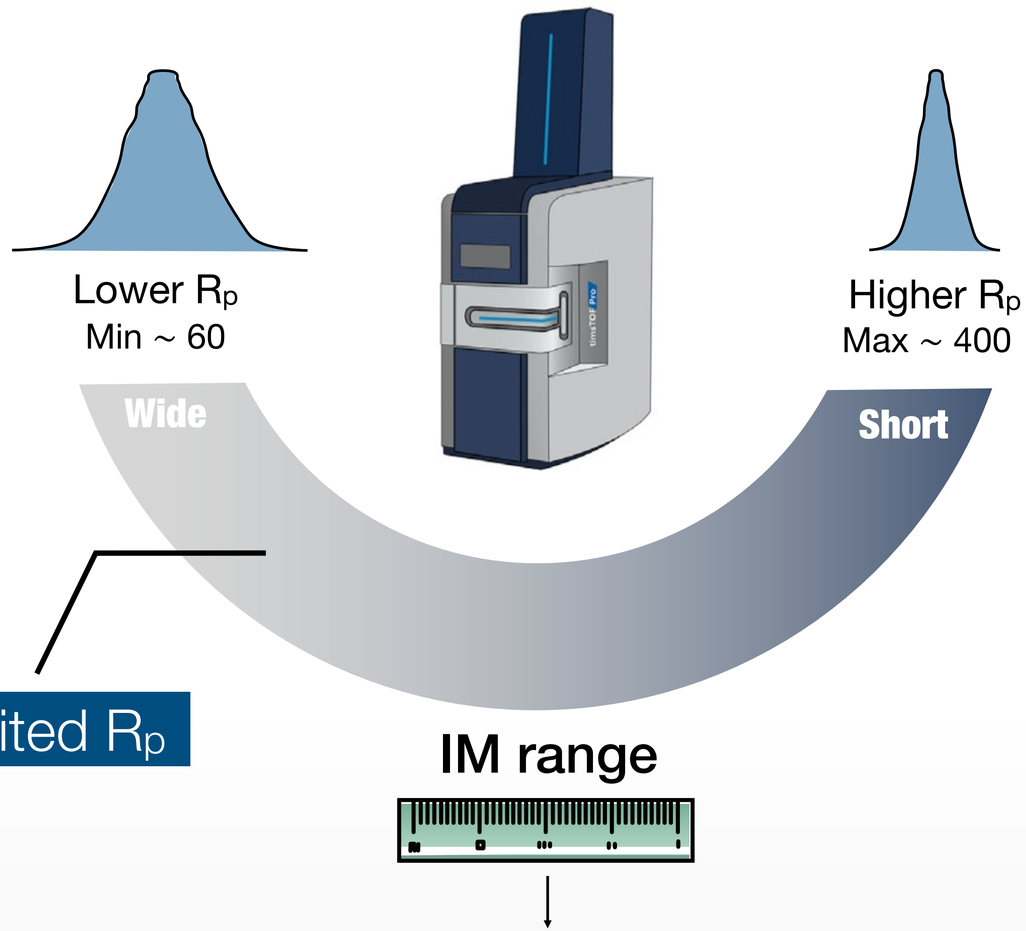
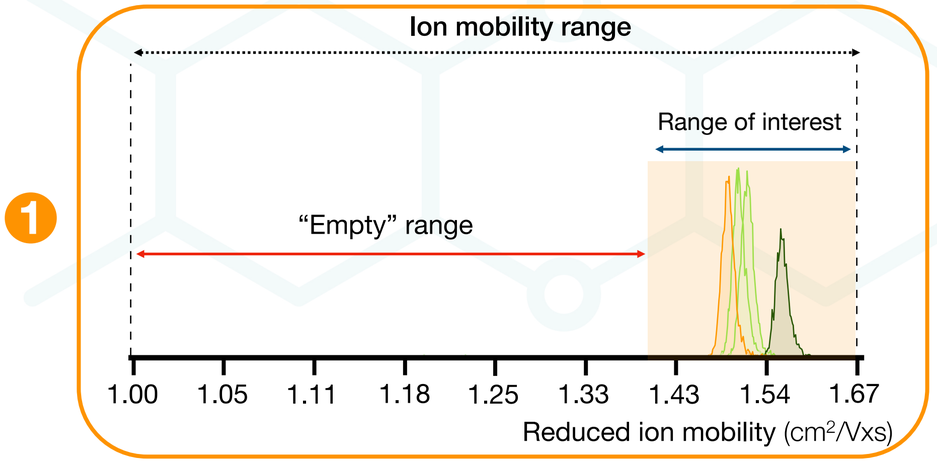
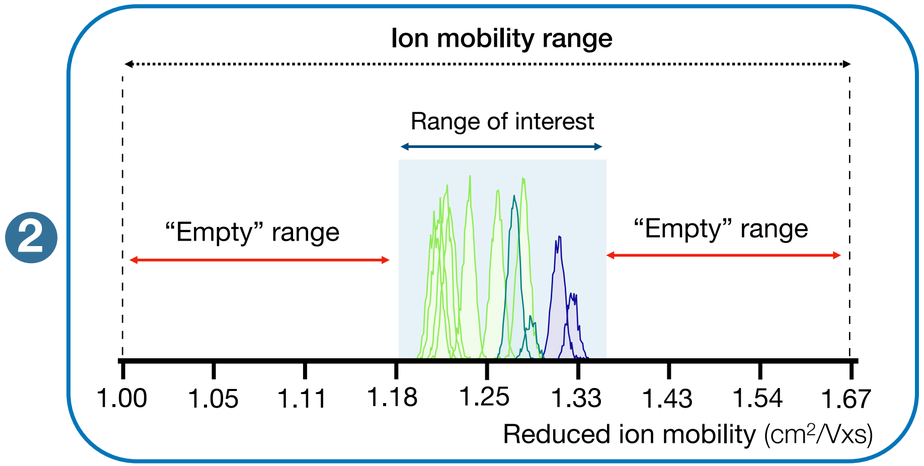
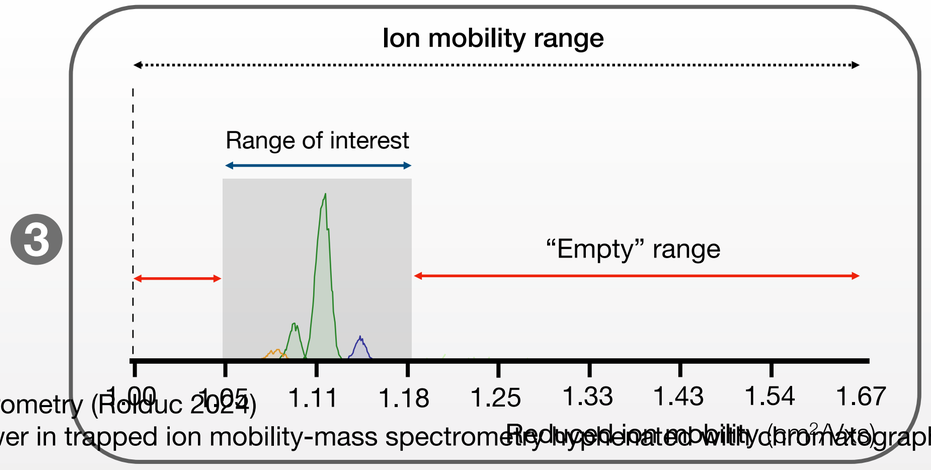
Standard mode



Can be **changed** during GC separation!







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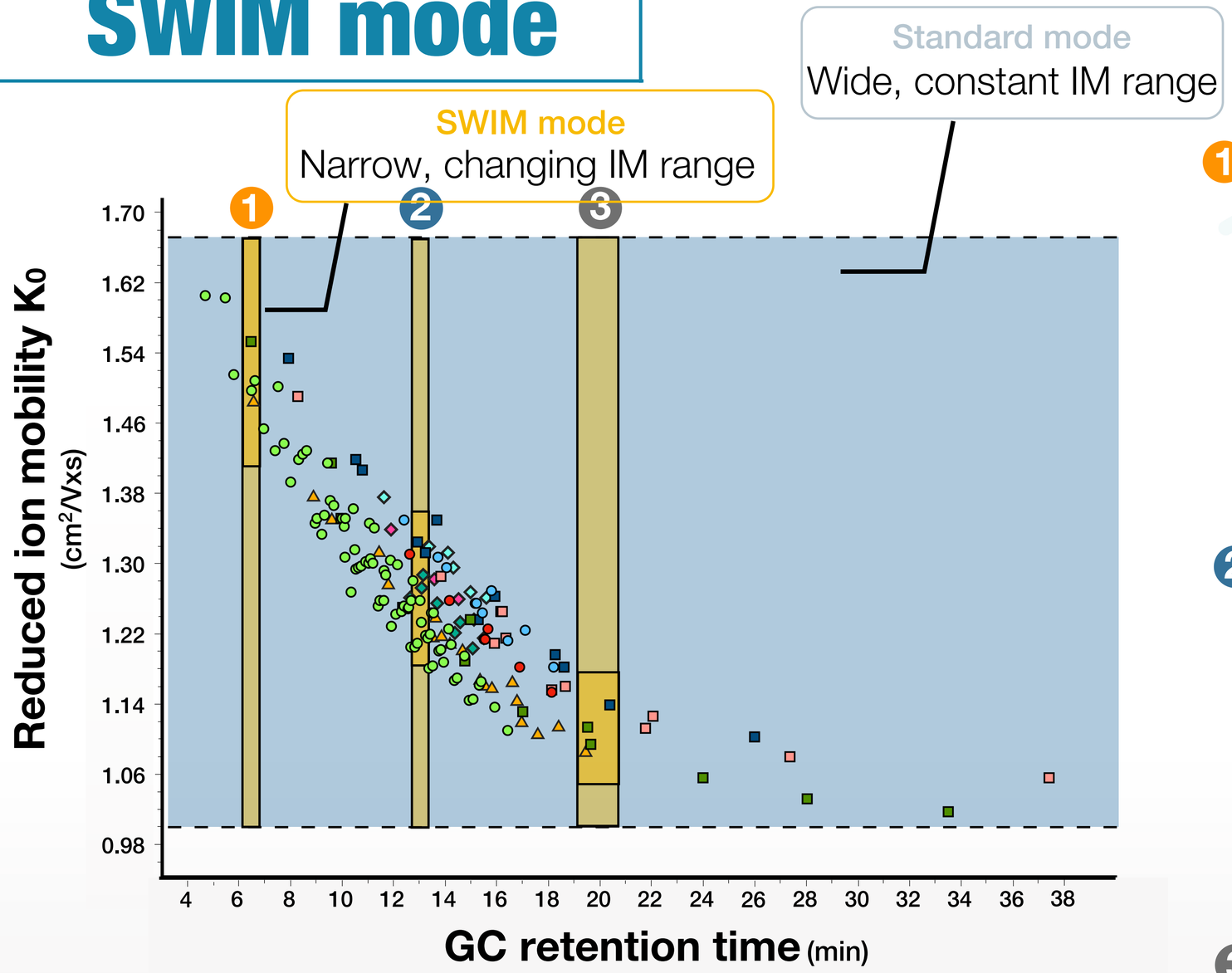
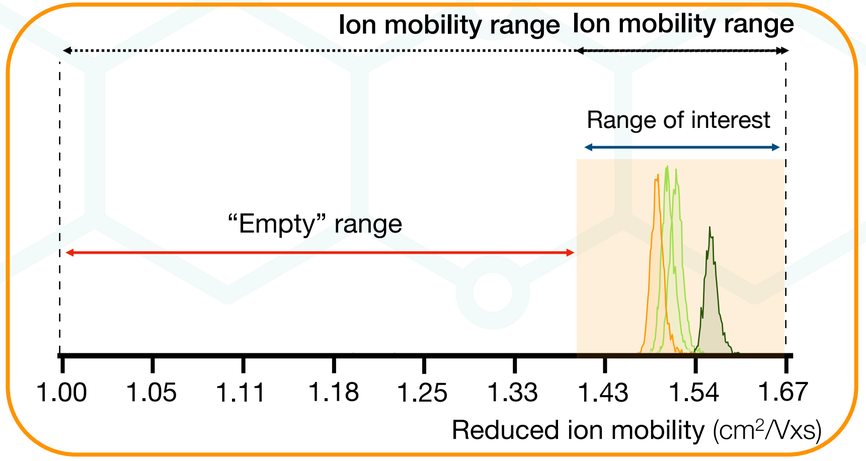
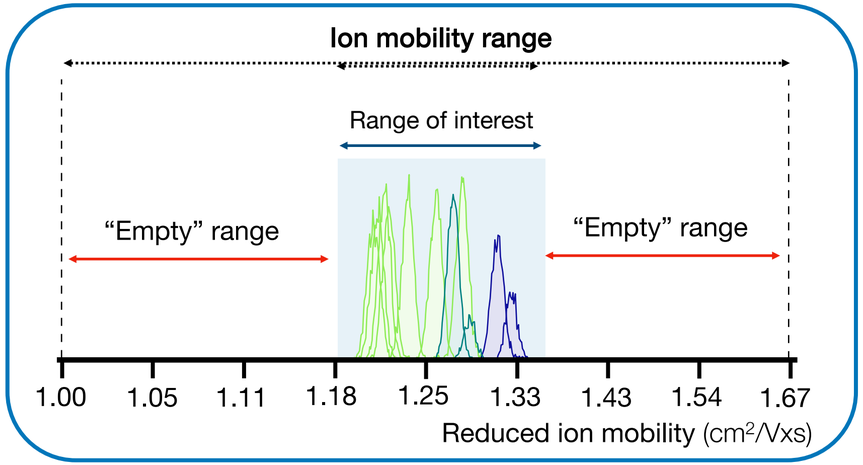
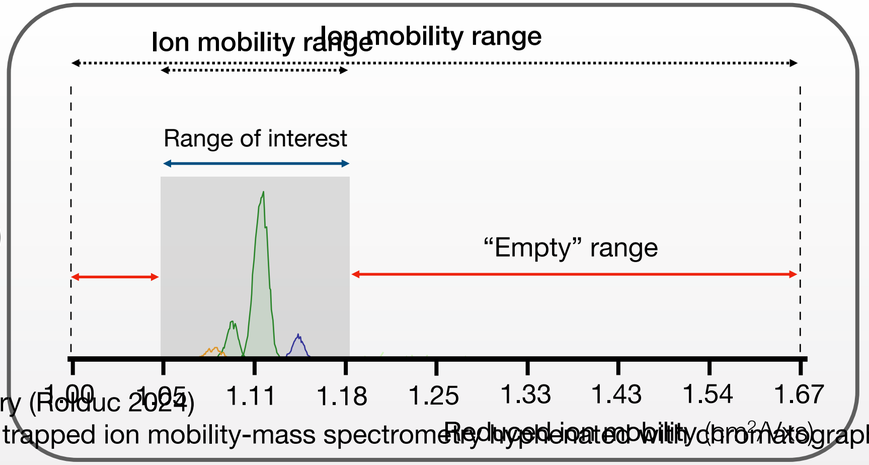
SWIM mode









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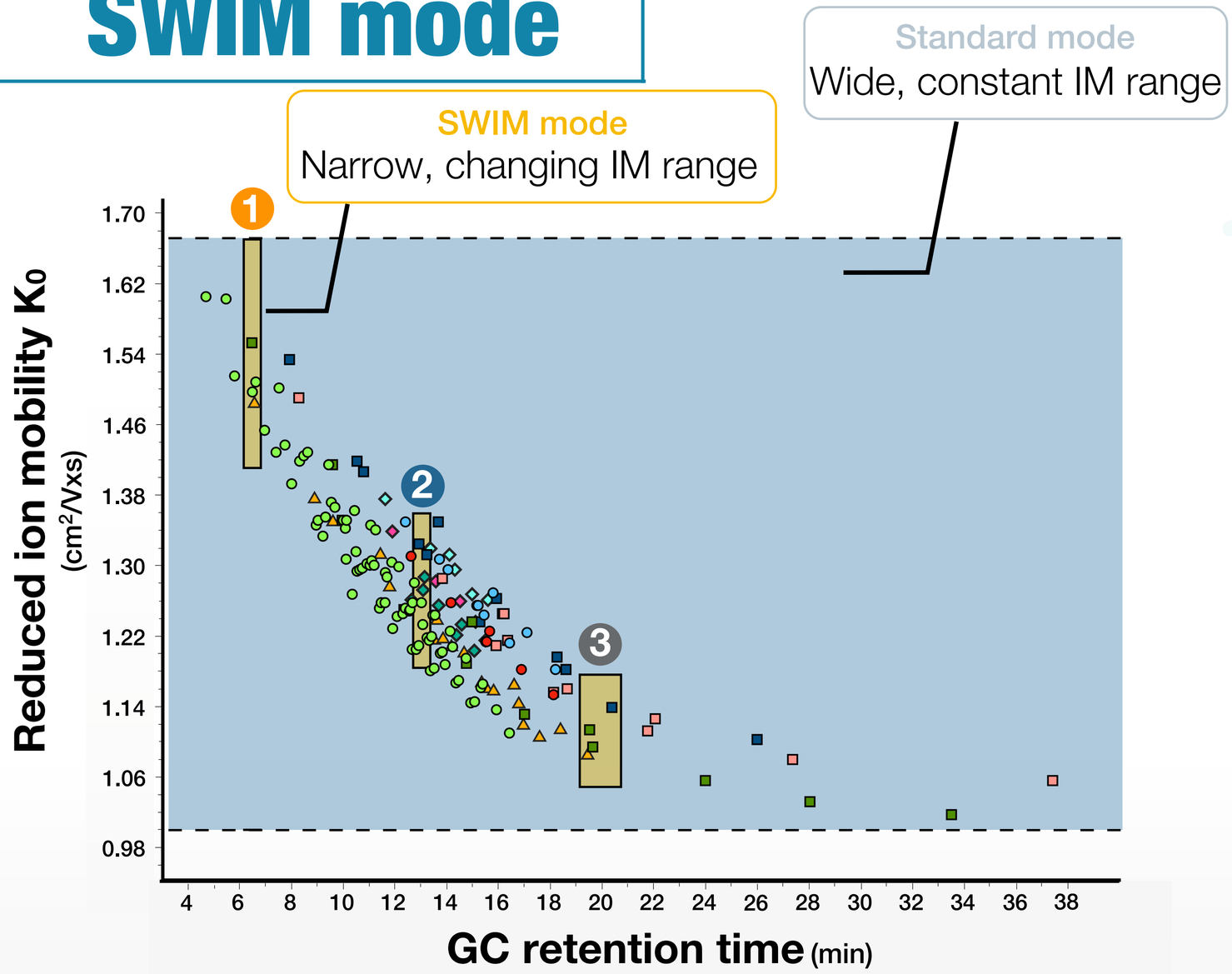
SWIM mode



Sliding

Windows

Ion

Mobility

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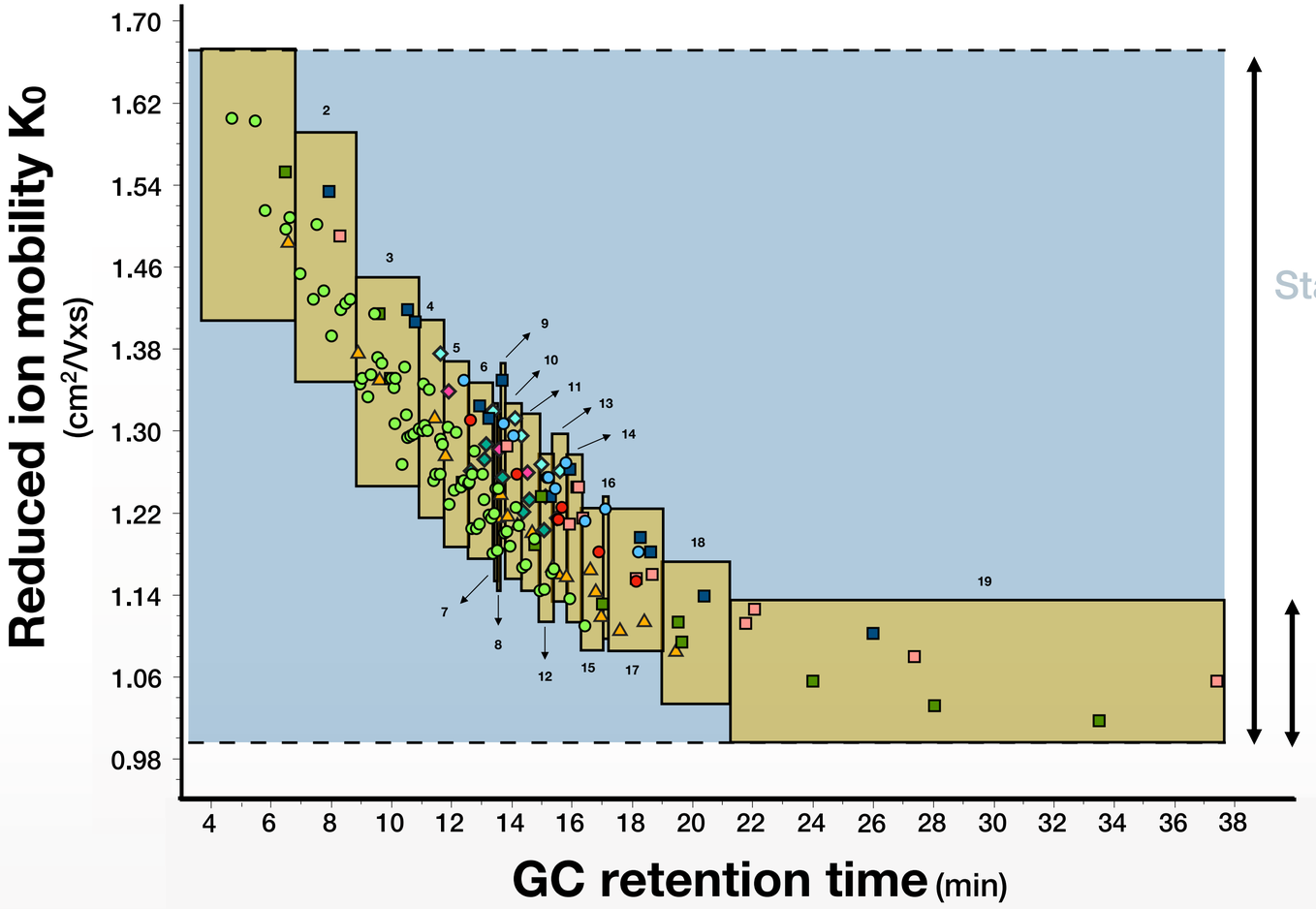
SWIM mode



Standard mode

SWIM mode
~ 4x smaller

Sliding
Windows
Ion
Mobility

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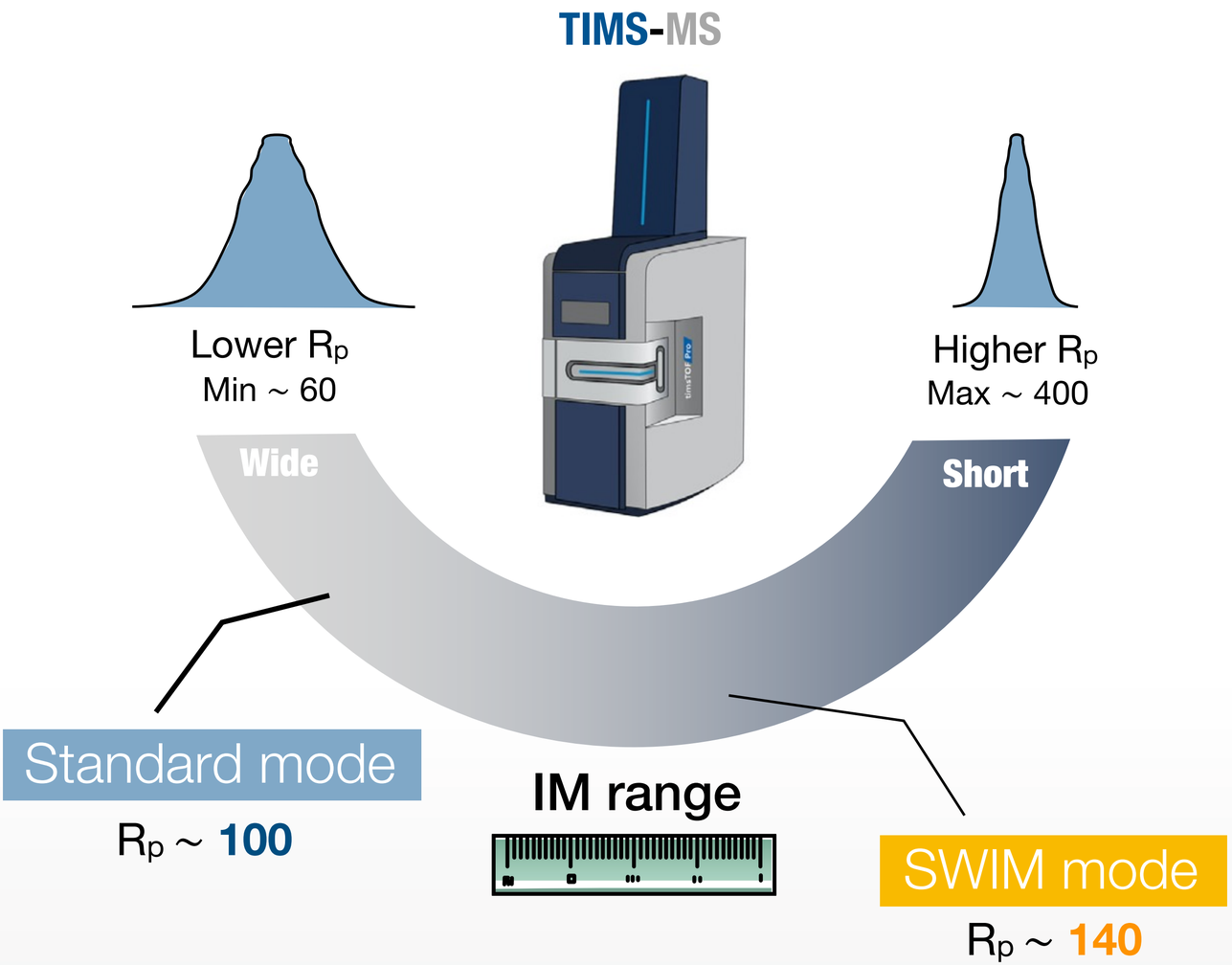
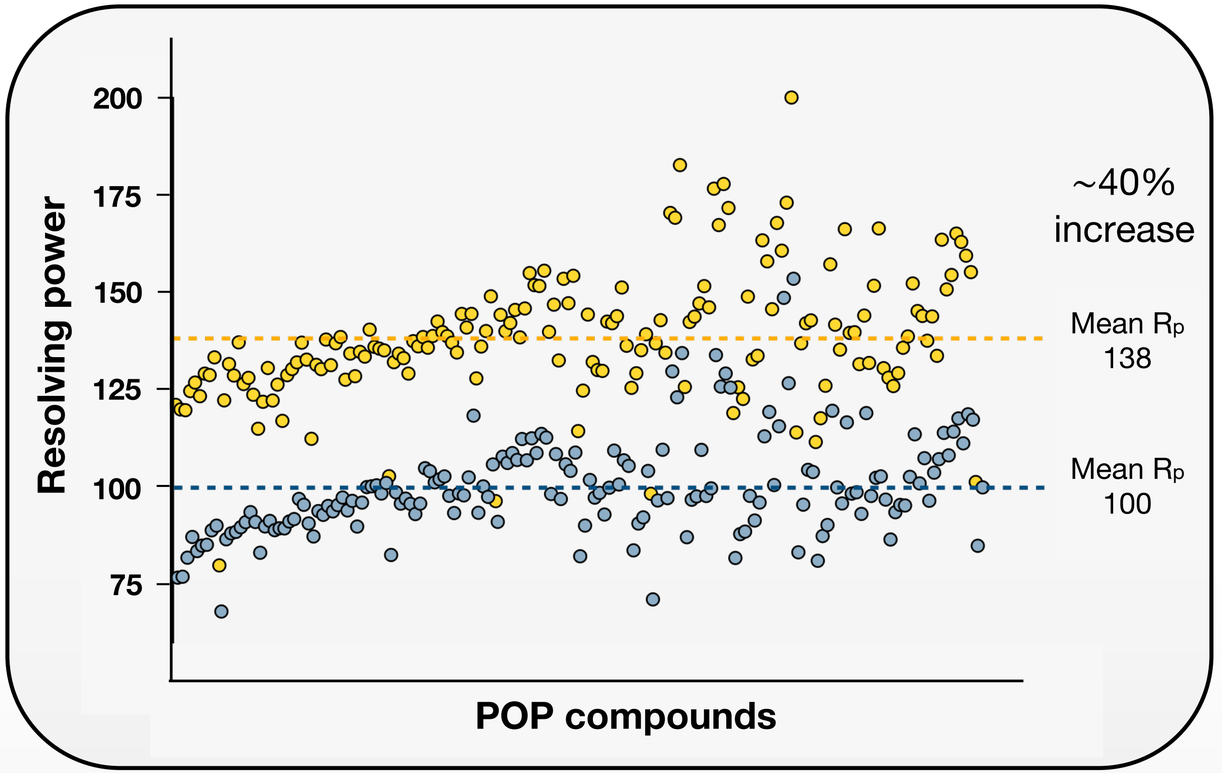
Rp improvement





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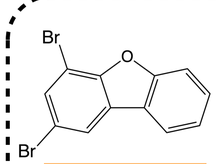
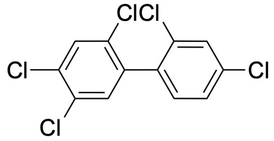
Selectivity improvement



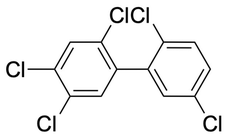
2,4-DiBDF

m/z 325.87**60**



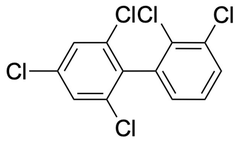
PeCB 90

m/z 325.87**99**



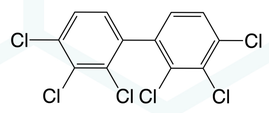
PeCB 101

m/z 325.87**99**



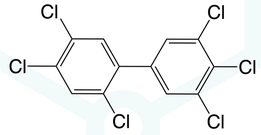
PeCB 84

m/z 325.87**99**



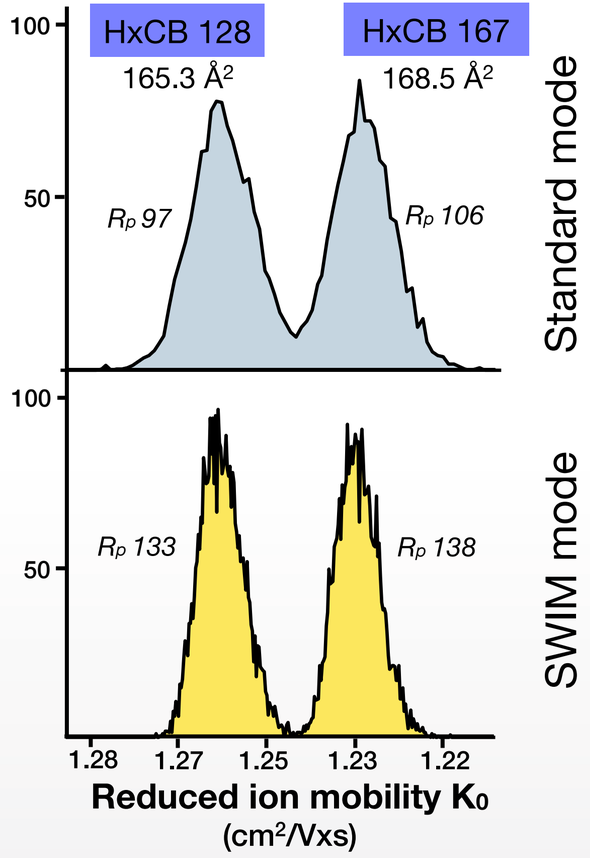
HxCB 128

m/z 359.8410



HxCB 167

m/z 359.8410



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Conclusion

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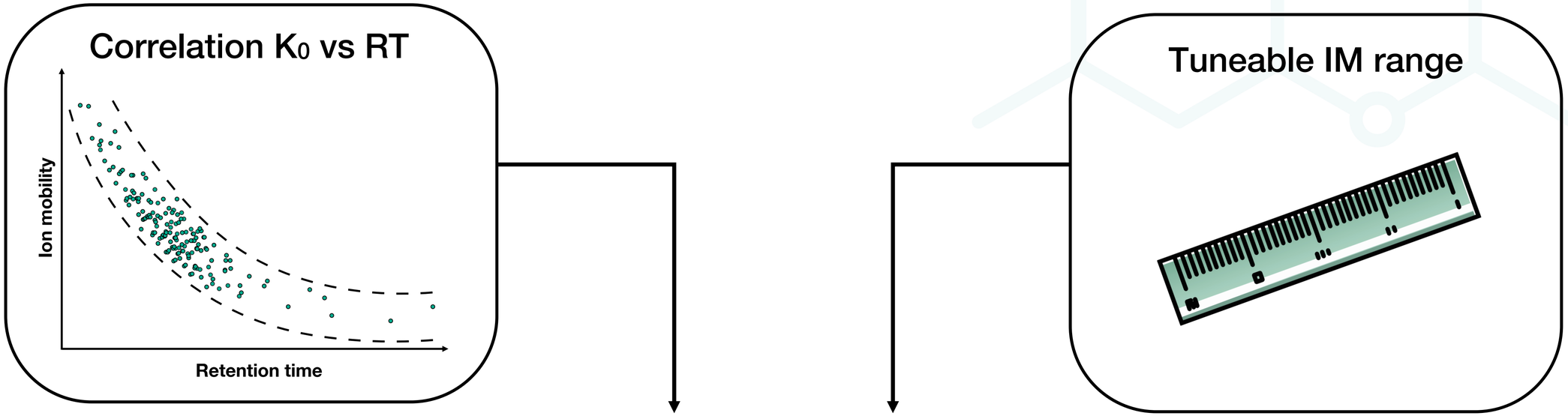
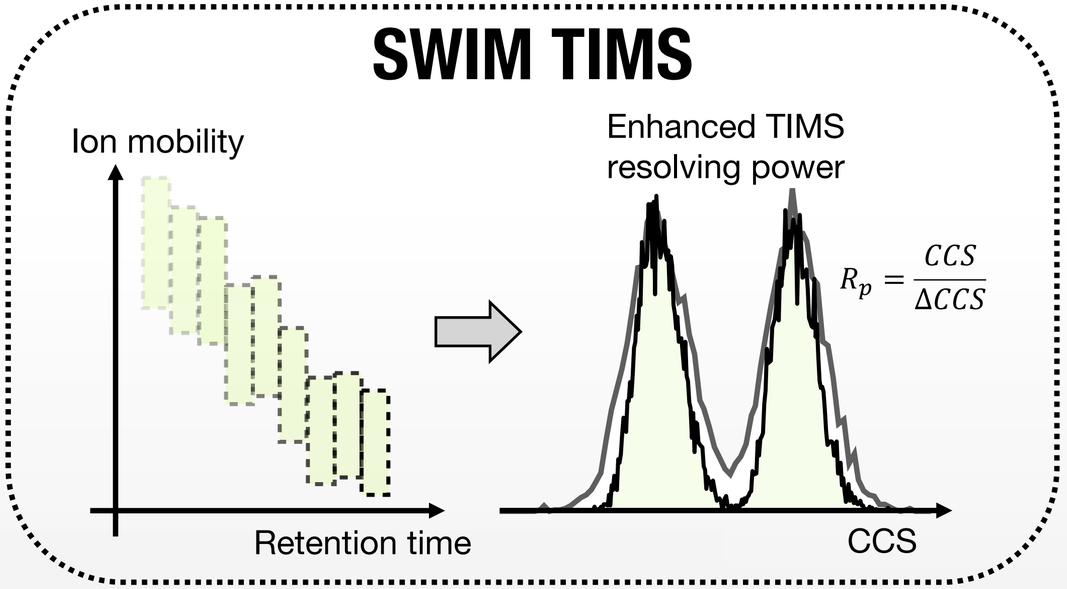
Summary





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Summary

analytical chemistry

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Hugo B. Muller, Georges Scholl, Johann Far, Edwin De Pauw, and Gauthier Eppe*

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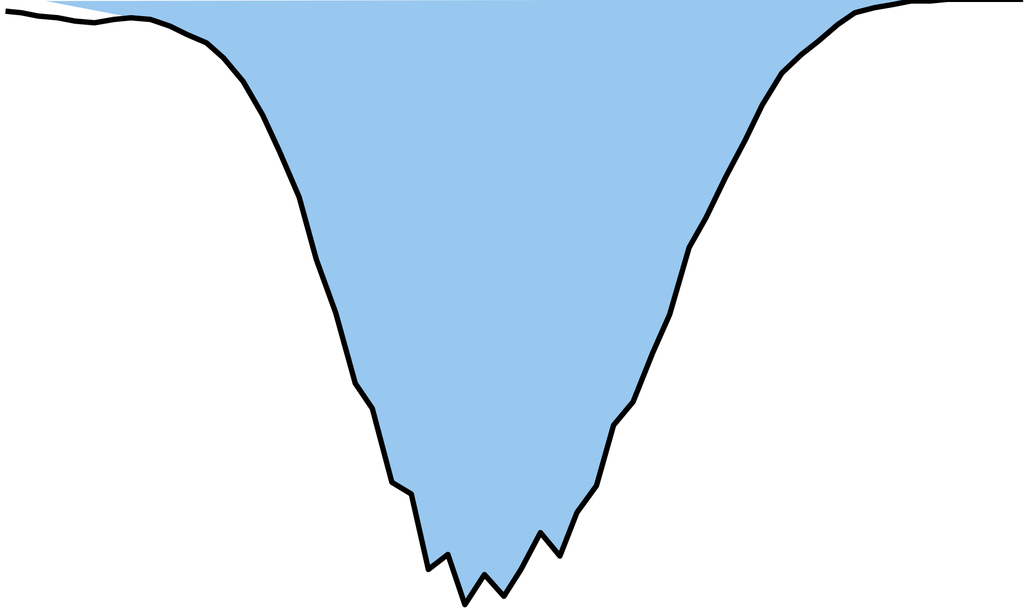

Thank you