DioXin 2023

10-14 SEPTEMBER **MAASTRICHT, THE NETHERLANDS**

43rd International Symposium on
Halogenated Persistent Organic Pollutants

DioXin 2023

10-14 SEPTEMBER MAASTRICHT, THE NETHERLANDS

LIÈGE université

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

Hugo Muller
PhD student

Monday, 10 September 2023

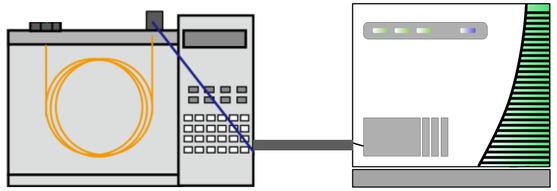
MASS LABORATORY SPECTROMETRY

Introduction

LIÈGE université

POPs analysis in food

Traditional approach



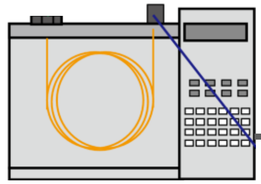
GC

Separates neutrals according to **boiling point**

MS

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

Our approach



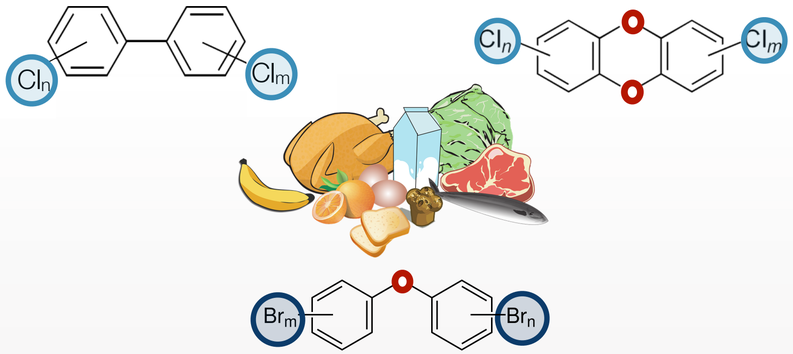
GC

Boiling point

Ion Mobility-MS

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

m/z ratio



Hugo 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”

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 constant

Fundamental low-field mobility equation

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

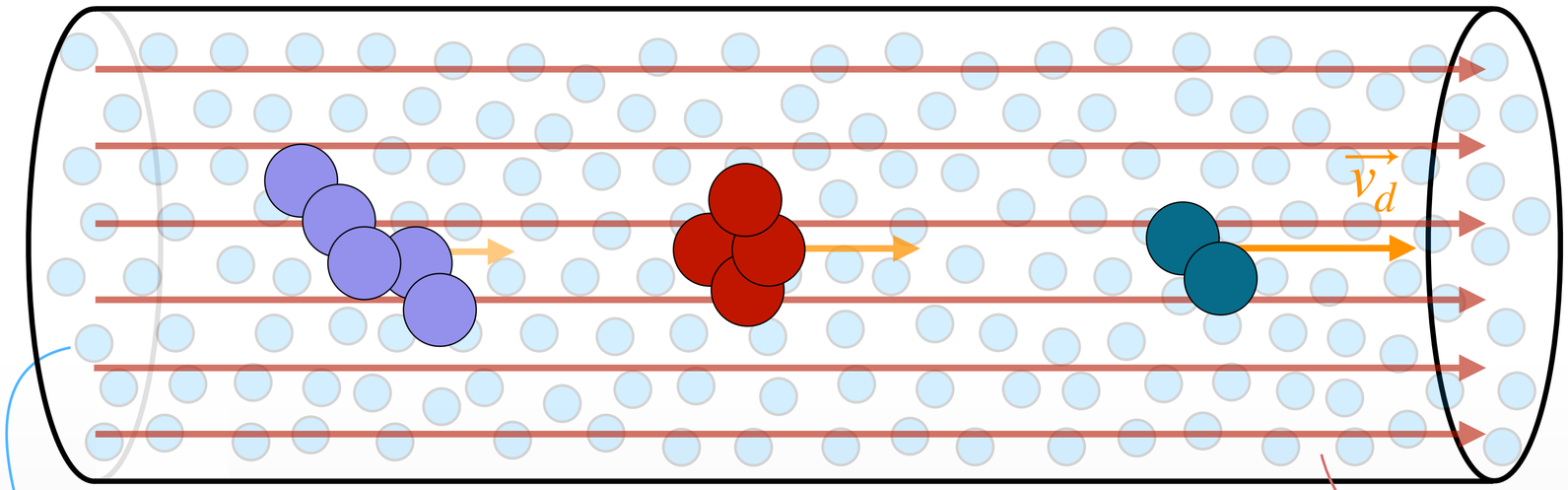
Charge

Mass

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

Size & shape

Ion-gas interaction potential



Drift gas (N_2)

Electric field $\vec{E}$

Hugo 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"

Ion mobility

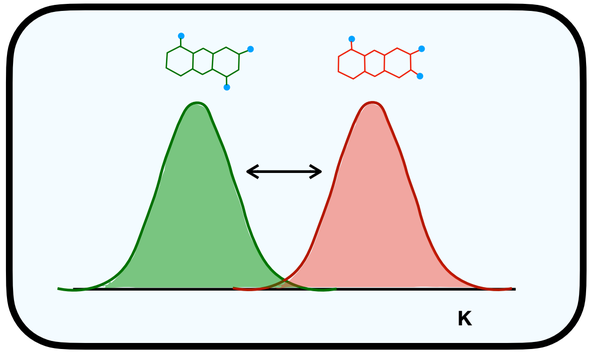
Technologies

- DTIMS
- TWIMS
- FAIMS/DMS
- TIMS

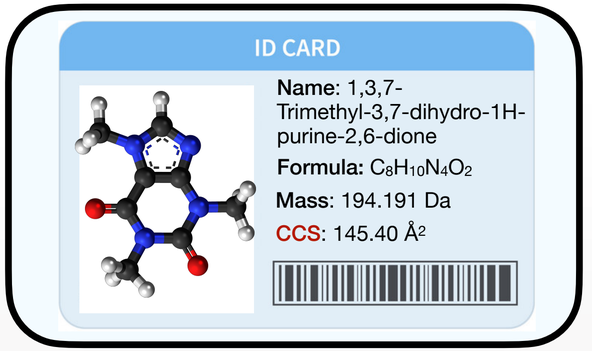
Ion mobility - mass spectrometry (IM-MS)

Advantages

- **Selectivity**
  - Isomers & Isobars
  - Interferences



- **Specificity** — CCS



Hugo 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”

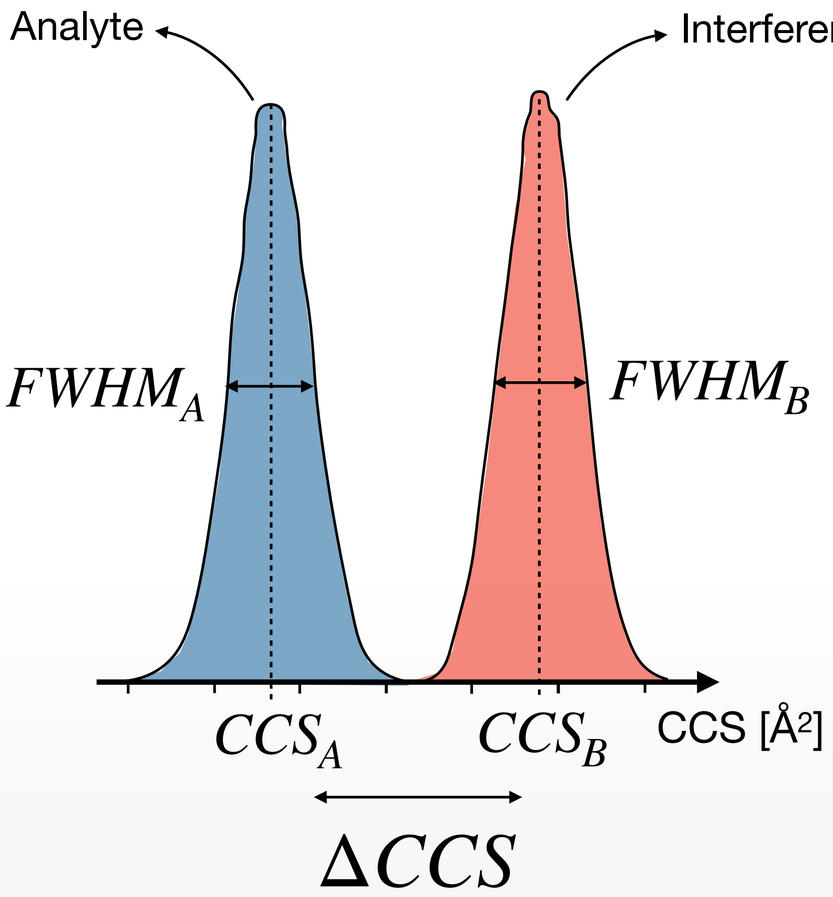
MASS SPECTROMETRY LABORATORY

Resolving power in IM

LIÈGE université

Resolving power

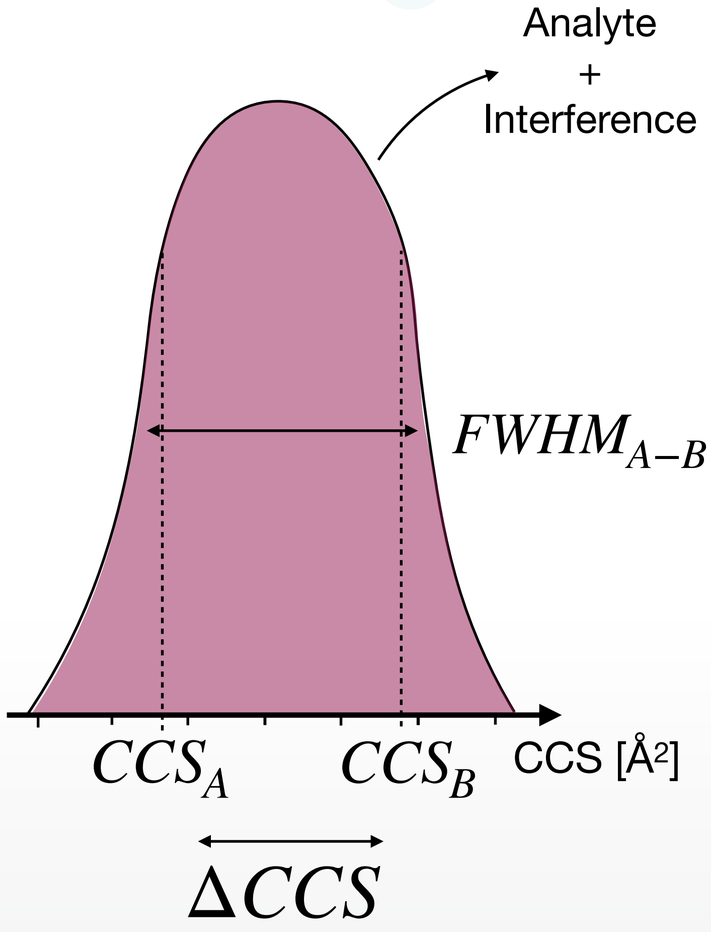
High resolving power



Resolving power

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

Low resolving power

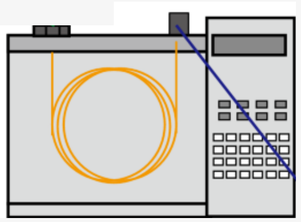


Hugo Muller et. al, “Sliding windows in ion mobility (SWIM): a new approach to increase the separation power in trapped ion mobility-mass spectrometry hyphenated with chromatography”

Rp in TIMS

Analysis time

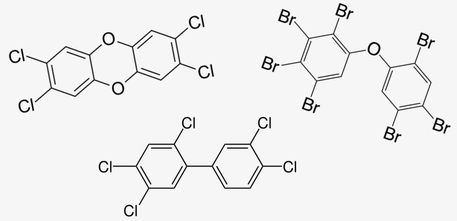
GC coupling



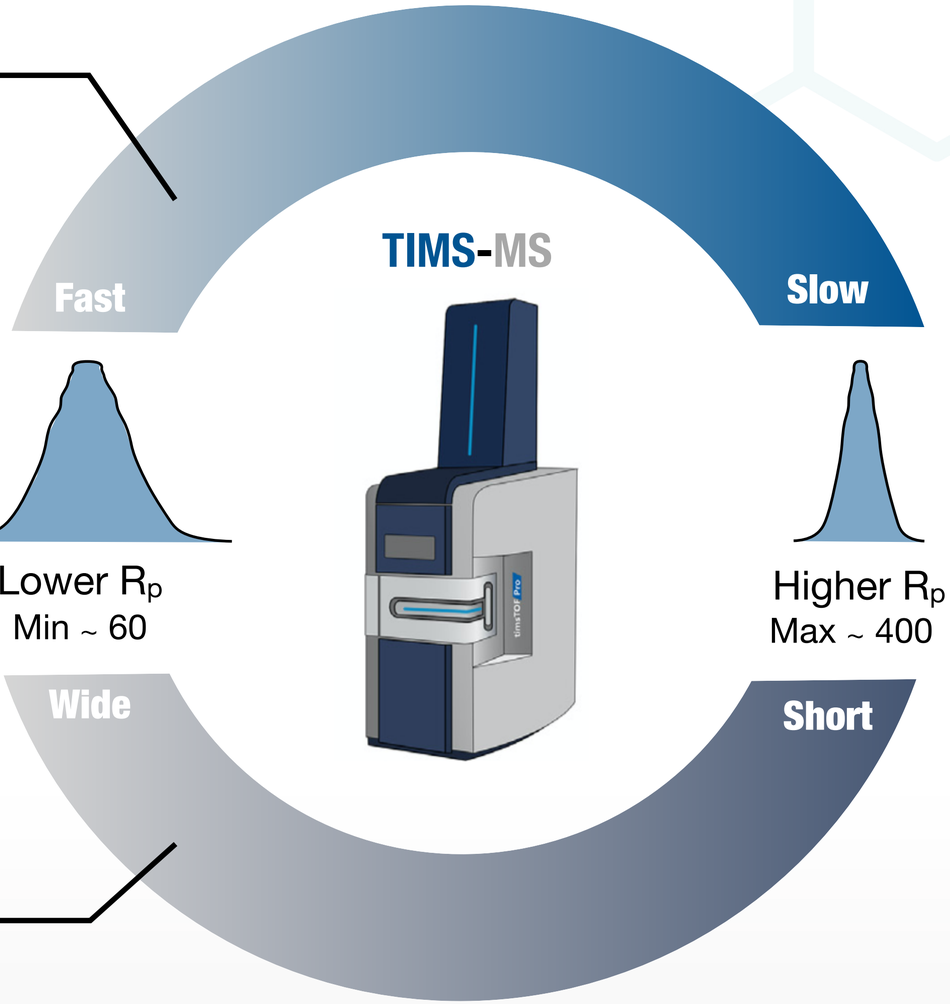
⇒ Fast IM separations

Limited R_p

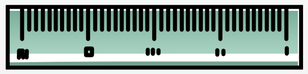
Diversity of POPs



⇒ Wide IM range



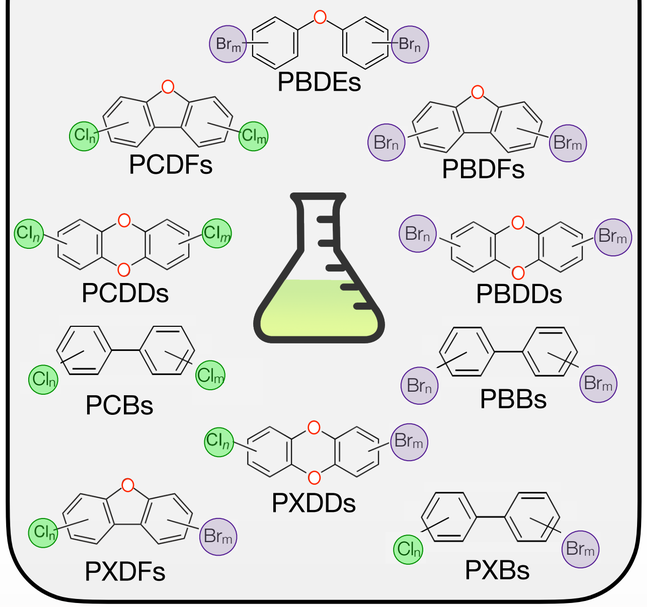
IM range



Hugo 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”

Rp in TIMS

Mixture of 174 POP standards

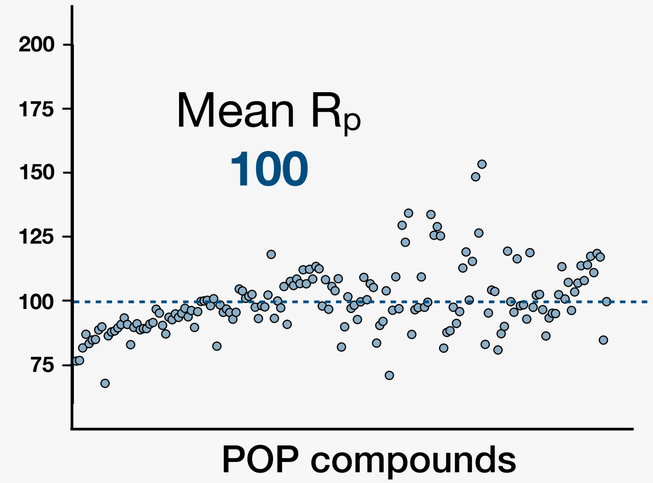


GC-TIMS-MS analysis

Analysis time:
350 ms

IM range:
1.00 - 1.67 K_0

Resolving power



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

Hugo 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”

MASS SPECTROMETRY LABORATORY

SWIM

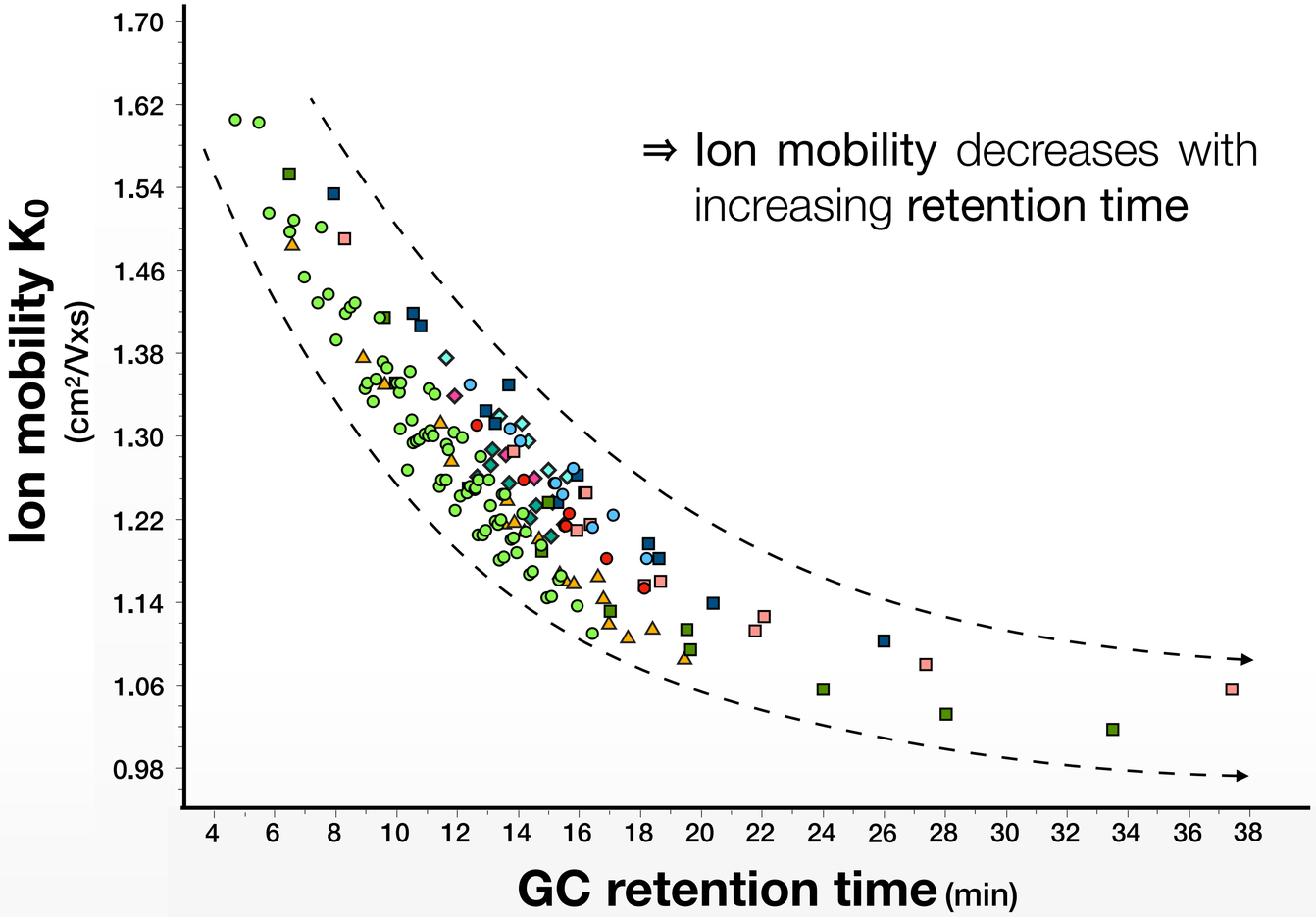
Sliding Windows in Ion Mobility

LIÈGE université

Dioxin 2023
10-14 SEPTEMBER MAASTRICHT, THE NETHERLANDS

43rd International Symposium on Halogenated Persistent Organic Pollutants (POPs)

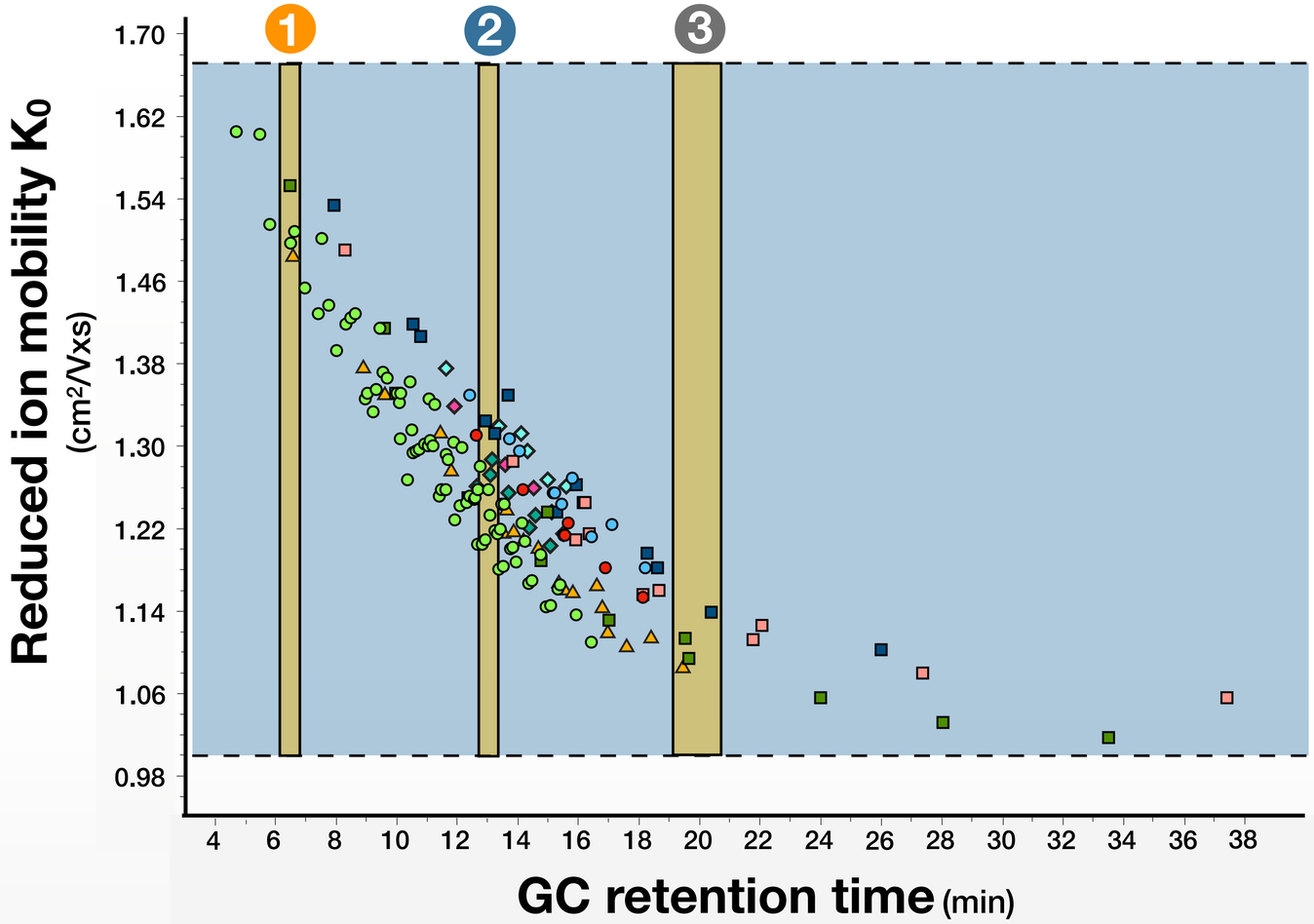
RT vs K correlation

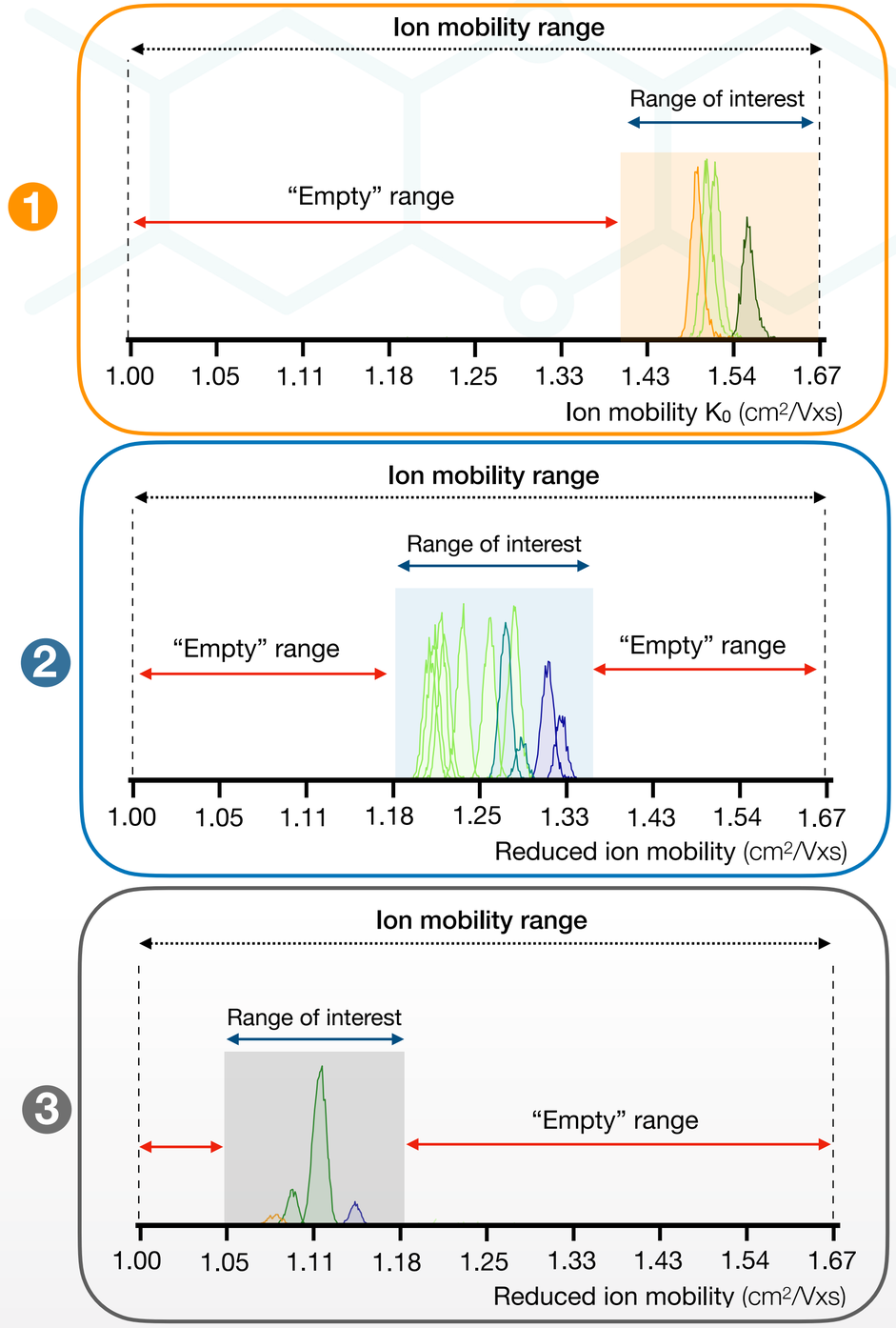


⇒ Ion mobility decreases with increasing **retention time**

Hugo 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”

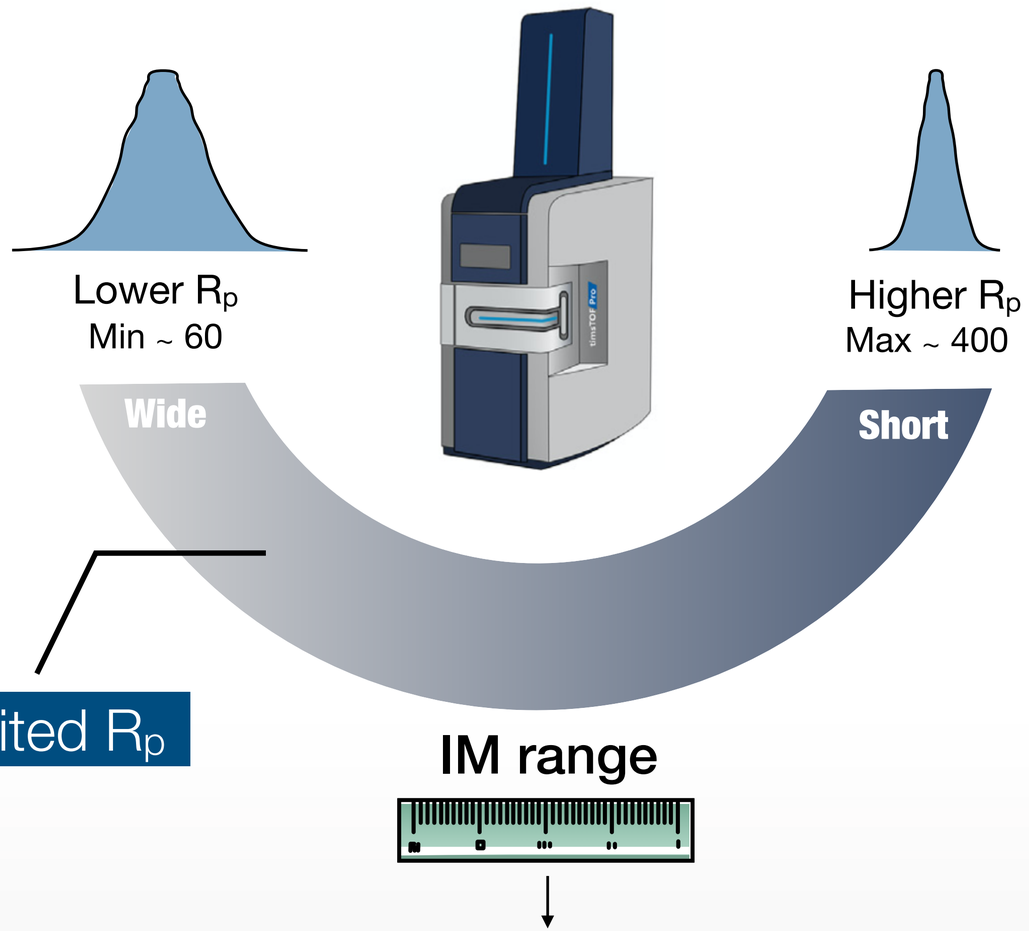
Standard mode



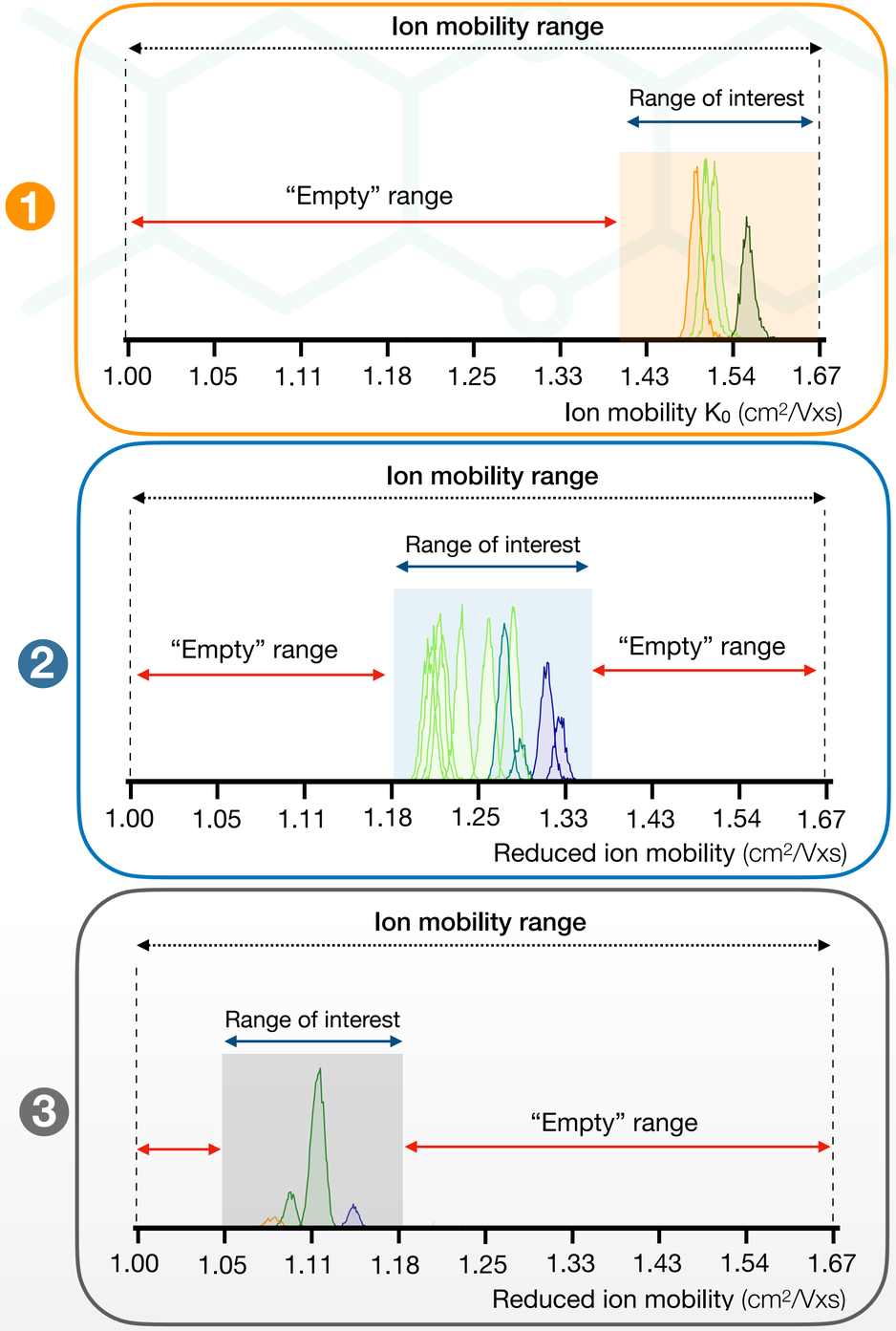


Hugo Muller et. al, "Sliding windows in ion mobility (SWIM): a new approach to increase the separation power in trapped ion mobility-mass spectrometry hyphenated with chromatography"

Standard mode



Can be **changed** during GC separation!

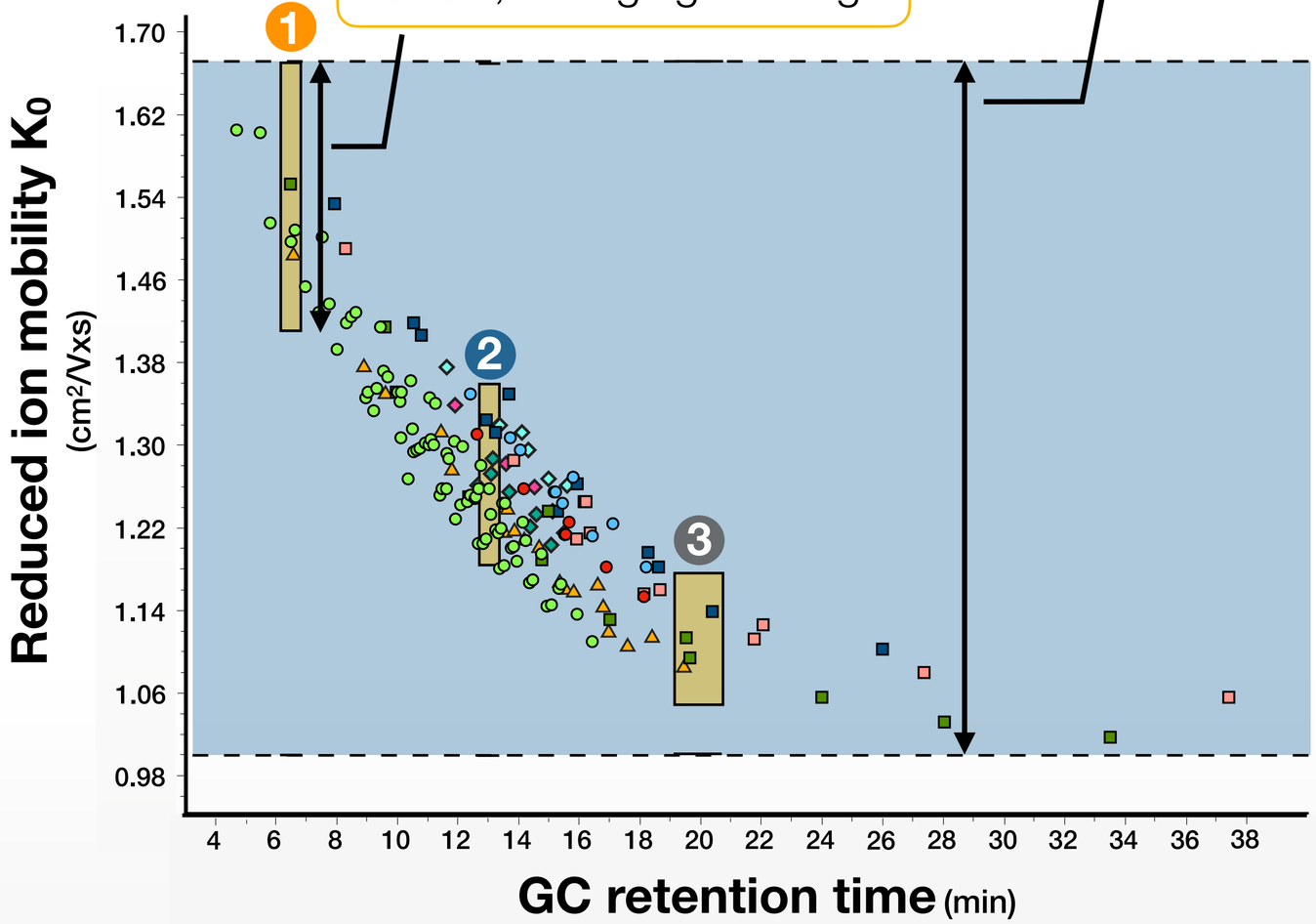


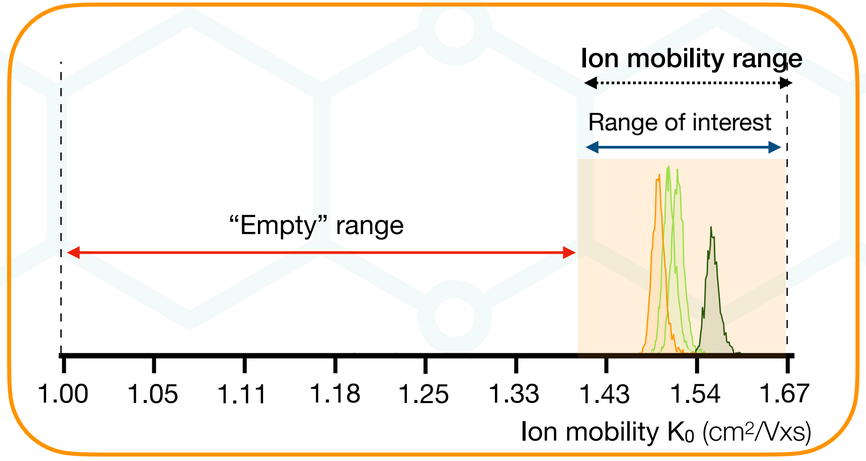
Hugo Muller et. al, "Sliding windows in ion mobility (SWIM): a new approach to increase the separation power in trapped ion mobility-mass spectrometry hyphenated with chromatography"

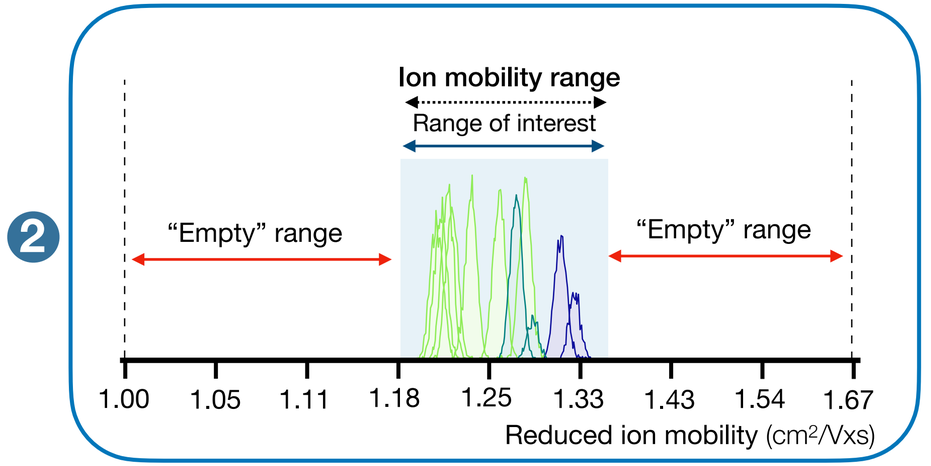
SWIM mode

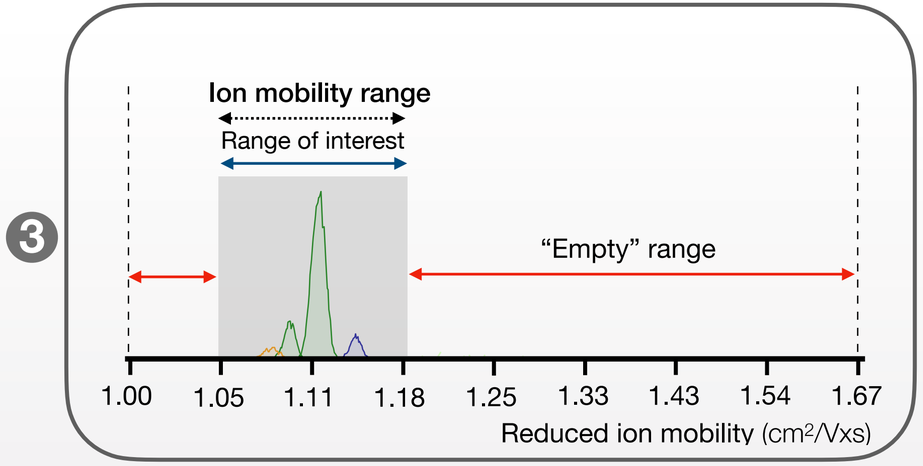
Standard mode
Wide, constant IM range

SWIM mode
Narrow, changing IM range



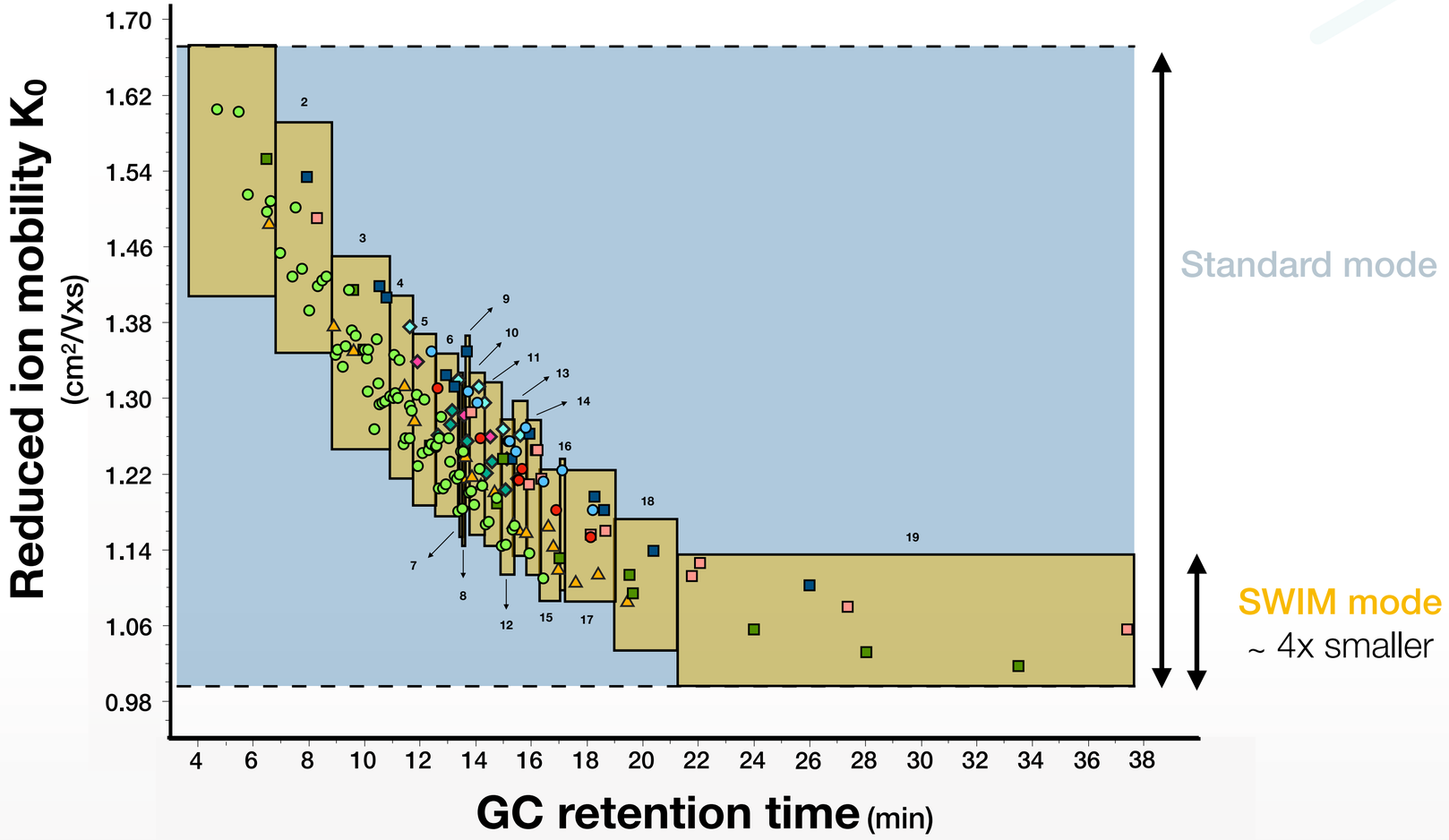






Hugo Muller et. al, "Sliding windows in ion mobility (SWIM): a new approach to increase the separation power in trapped ion mobility-mass spectrometry hyphenated with chromatography"

SWIM mode



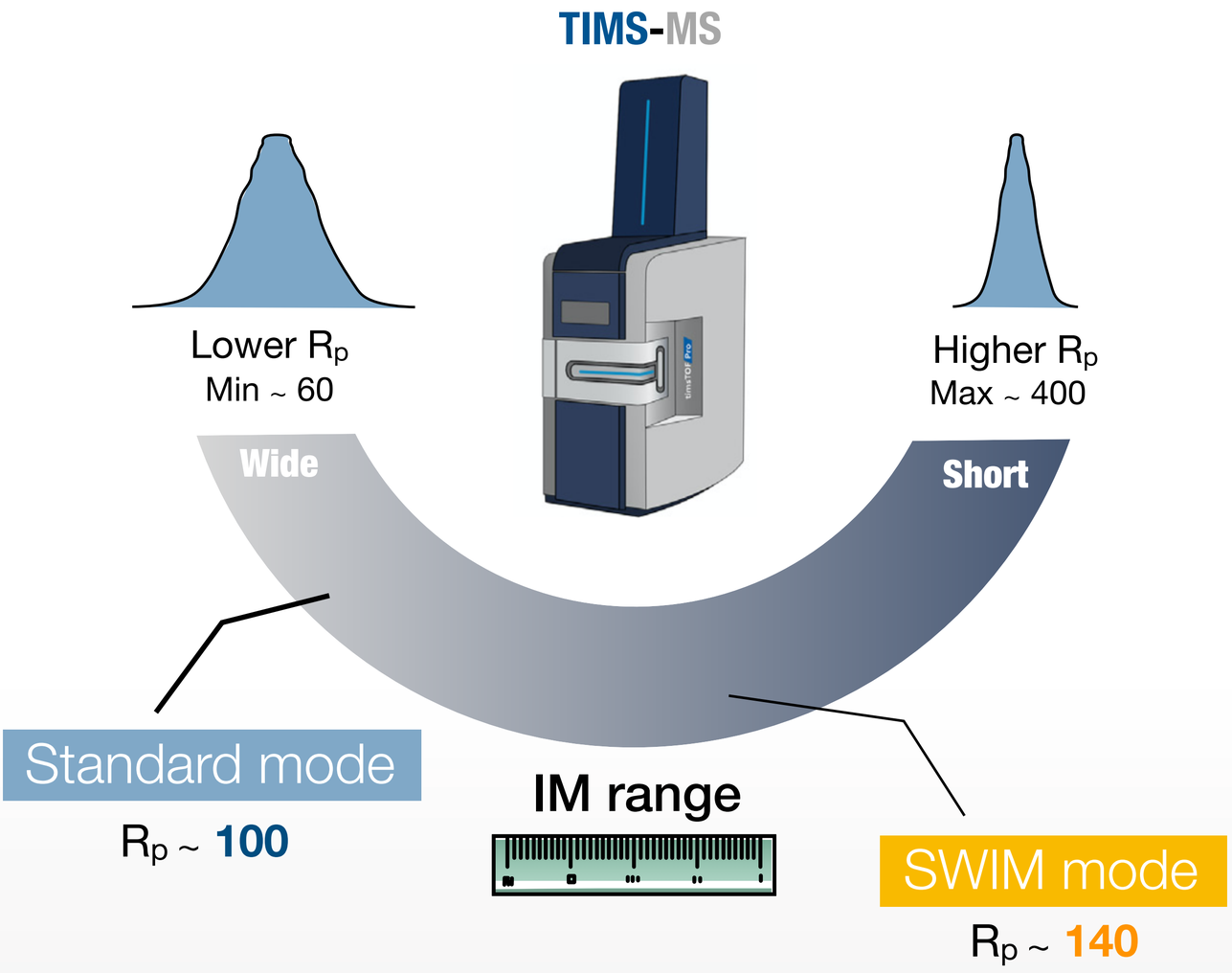
Standard mode

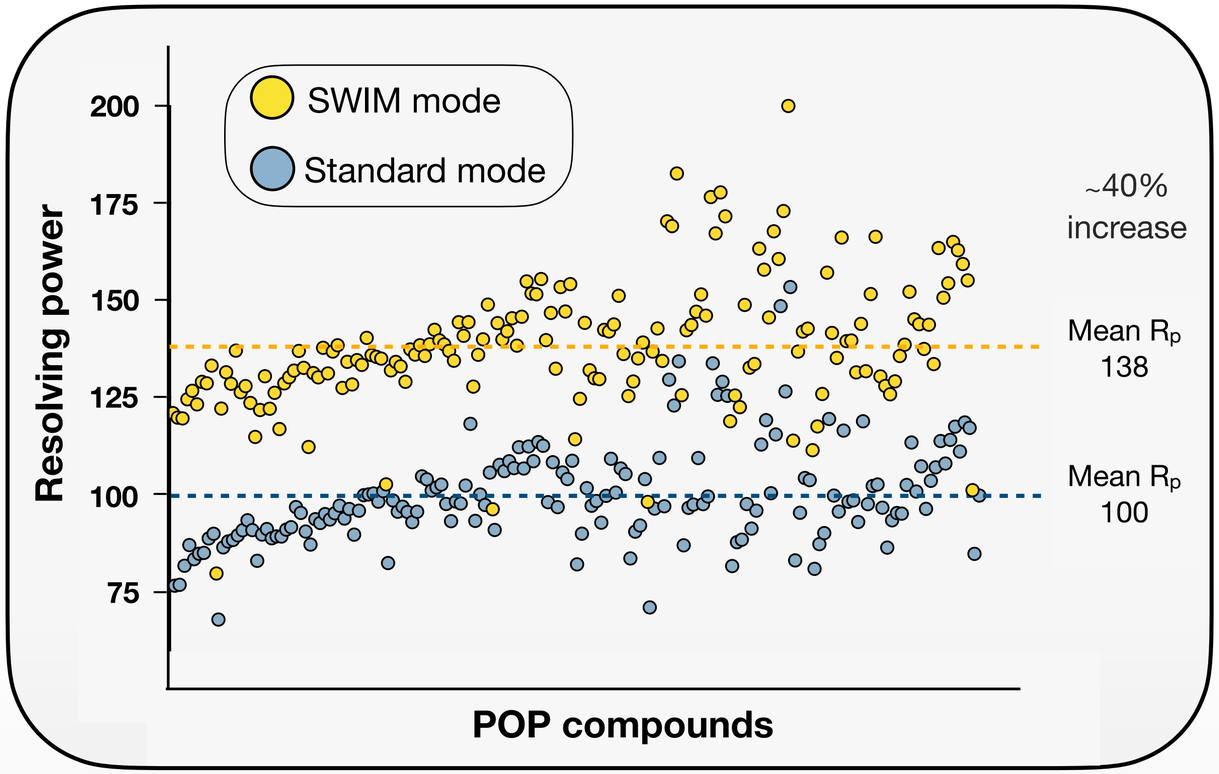
SWIM mode
~ 4x smaller

Sliding
Windows
Ion
Mobility

Hugo 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”

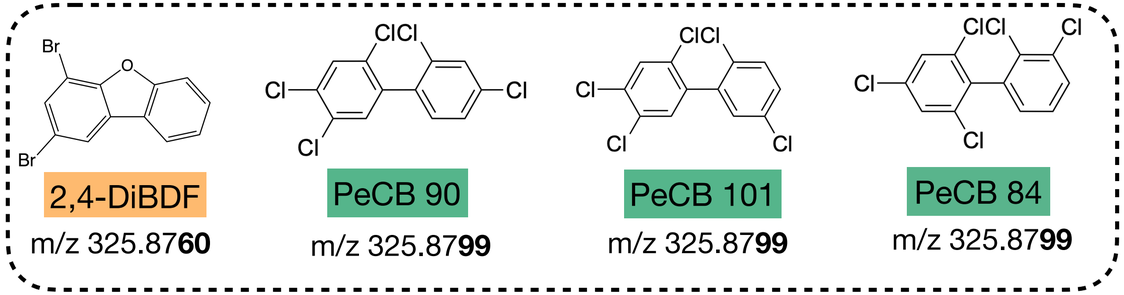
Rp improvement

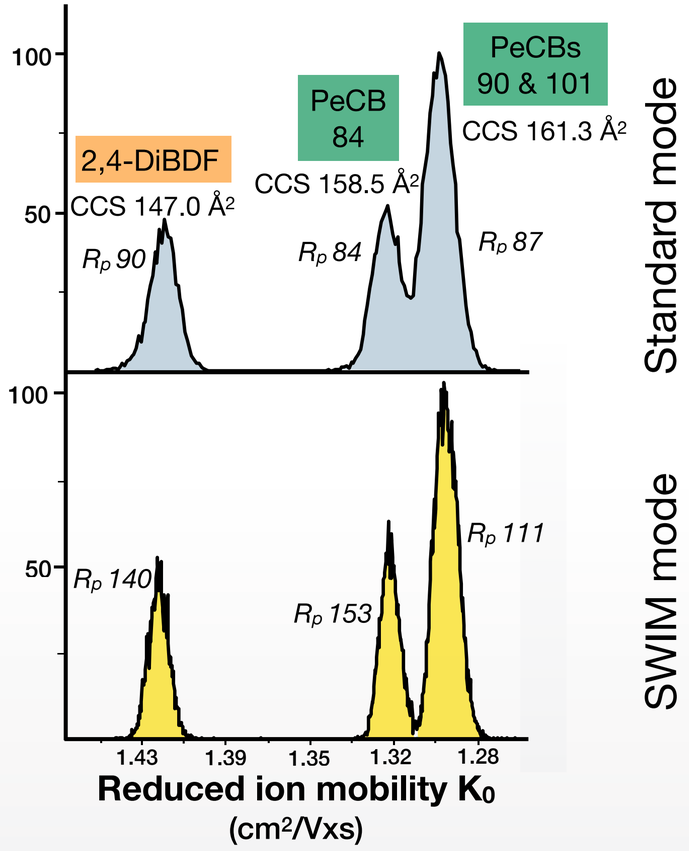


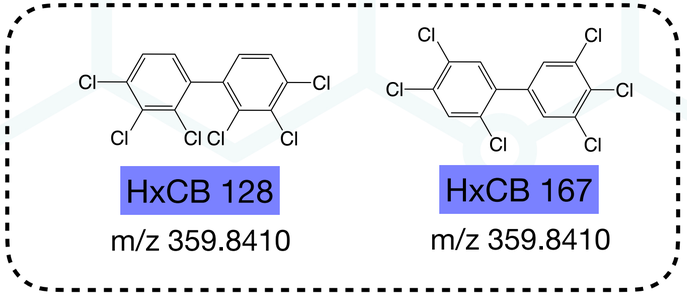


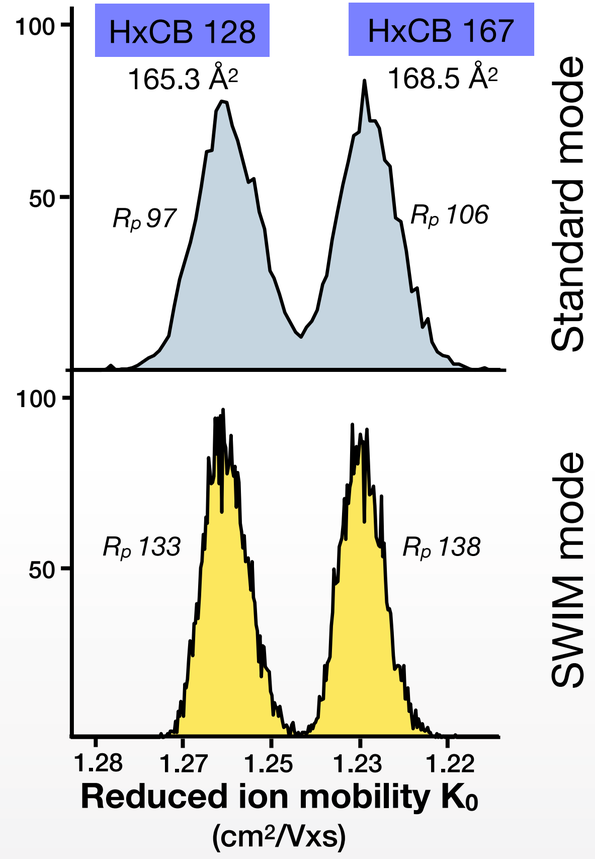
Hugo Muller et. al, “Sliding windows in ion mobility (SWIM): a new approach to increase the separation power in trapped ion mobility-mass spectrometry hyphenated with chromatography”

Selectivity improvement









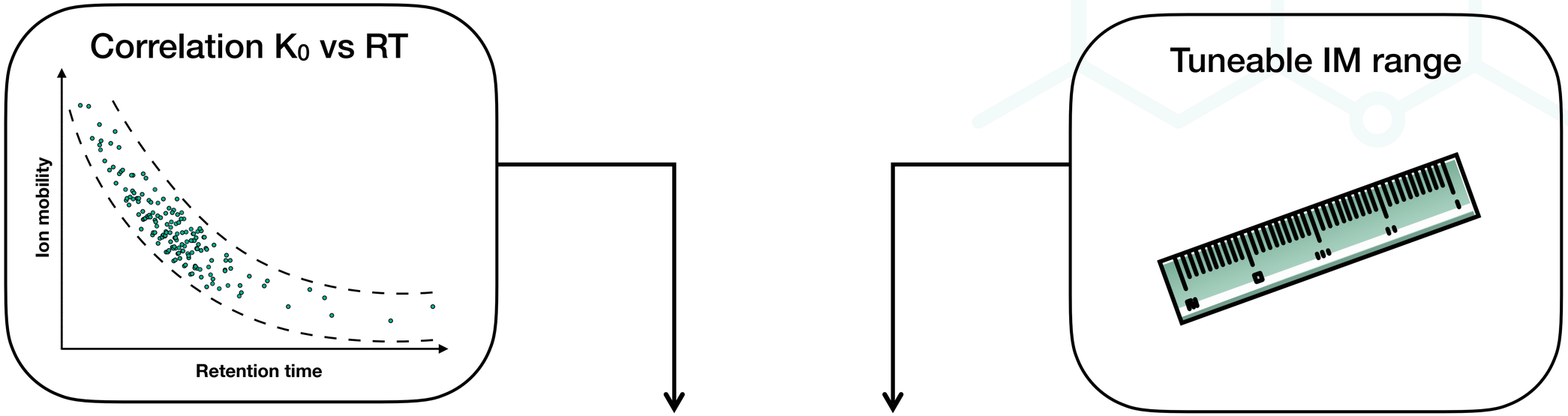
Hugo Muller et. al, “Sliding windows in ion mobility (SWIM): a new approach to increase the separation power in trapped ion mobility-mass spectrometry hyphenated with chromatography”

MASS SPECTROMETRY LABORATORY

Conclusion

LIÈGE université

Summary



Hugo 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”

Publication

analytical chemistry

pubs.acs.org/ac Article

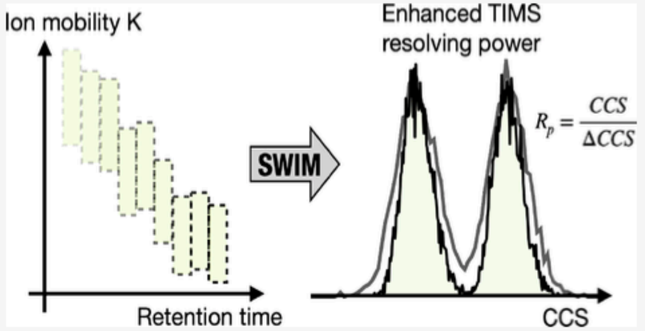
Sliding Windows in Ion Mobility (SWIM): A New Approach to Increase the Resolving Power in Trapped Ion Mobility-Mass Spectrometry Hyphenated with Chromatography

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

Cite This: *Anal. Chem.* 2023, 95, 17586–17594 Read Online

ACCESS | Metrics & More | Article Recommendations | Supporting Information

ABSTRACT: Over the past decade, the separation efficiency achieved by linear IMS instruments has increased substantially, with state-of-the-art IM technologies, such as the trapped ion mobility (TIMS), the cyclic traveling wave ion mobility (cTWIMS), and the structure for lossless ion manipulation (SLIM) platforms commonly demonstrating resolving powers in excess of 200. However, for complex sample analysis that require front end separation, the achievement of such high resolving power in TIMS is significantly hampered, since the ion mobility range must be broad enough to analyze all the classes of compounds of interest, whereas the IM analysis time must be short enough to cope with the time scale of the preseparation technique employed. In this paper, we introduce the concept of sliding windows in ion mobility (SWIM) for chromatography hyphenated TIMS applications that bypasses the need to use a wide and fixed IM range by using instead narrow and mobile ion mobility windows that adapt to the analytes' ion mobility during chromatographic separation. GC-TIMS-MS analysis of a mixture of 174 standards from several halogenated persistent organic pollutant (POP) classes, including chlorinated and brominated dioxins, biphenyls, and PBDEs, demonstrated that the average IM resolving power could be increased up to 40% when the SWIM mode was used, thereby greatly increasing the method selectivity for the analysis of complex samples.



https://doi.org/10.1021/acs.analchem.3c03039

MSSV LABORATORY
SPECTROMETRY

LIÈGE université

- Pr. Gauthier Eppe
- Georges Scholl
- Edwin de Pauw
- Johann Far
- Aurore Schneiders

fnrs
FREEDOM TO RESEARCH

Thank you

Hugo Muller et. al, “Sliding windows in ion mobility (SWIM): a new approach to increase the separation po… …s spectrometry hyphena… …raphy”