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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

ISIMS 2023

32nd International Conference on Ion Mobility Spectrometry

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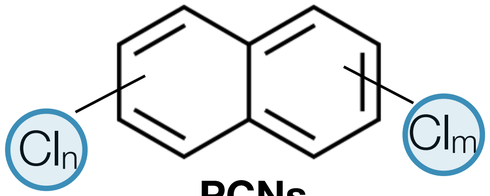
Introduction

POPs

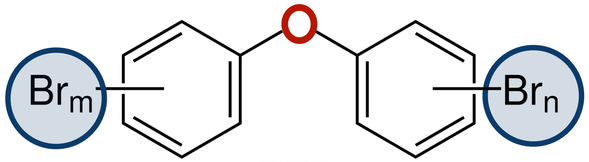
Persistent **o**rganic **p**ollutants

- → Toxic
- → Persistent
- → Bioaccumulative



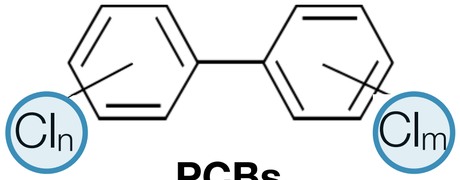
PCNs

Poly**c**hlorinated **N**aphtalenes



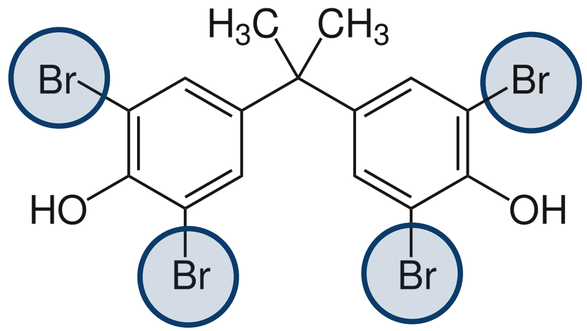
BFRs

Brominated **f**lame **r**etardants



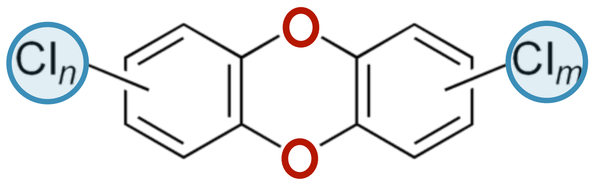
PCBs

Poly**c**hlorinated **B**iphenyls

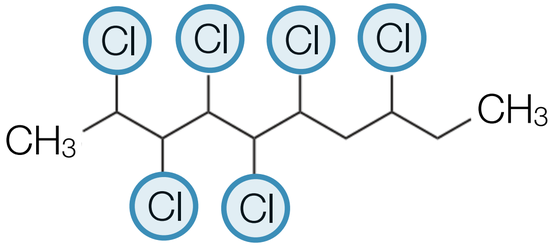


eBFRs

Emerging **BFRs**

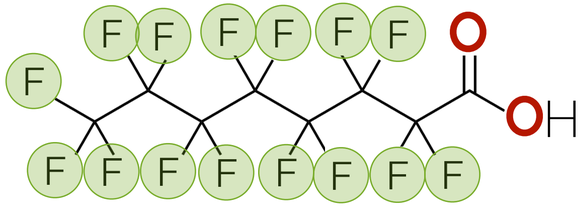


Dioxins



CPs

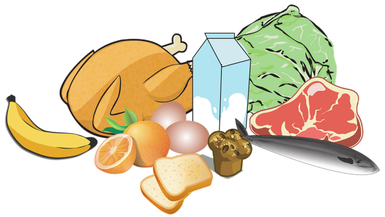
Chlorinated **p**araffins



PFAS

Perfluoroalkyl substances

Food consumption = major pathway of human exposure to most POPs



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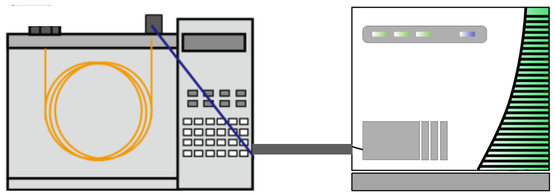
Analysis in food

Traditional approach



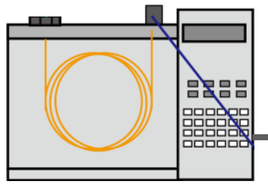
GC

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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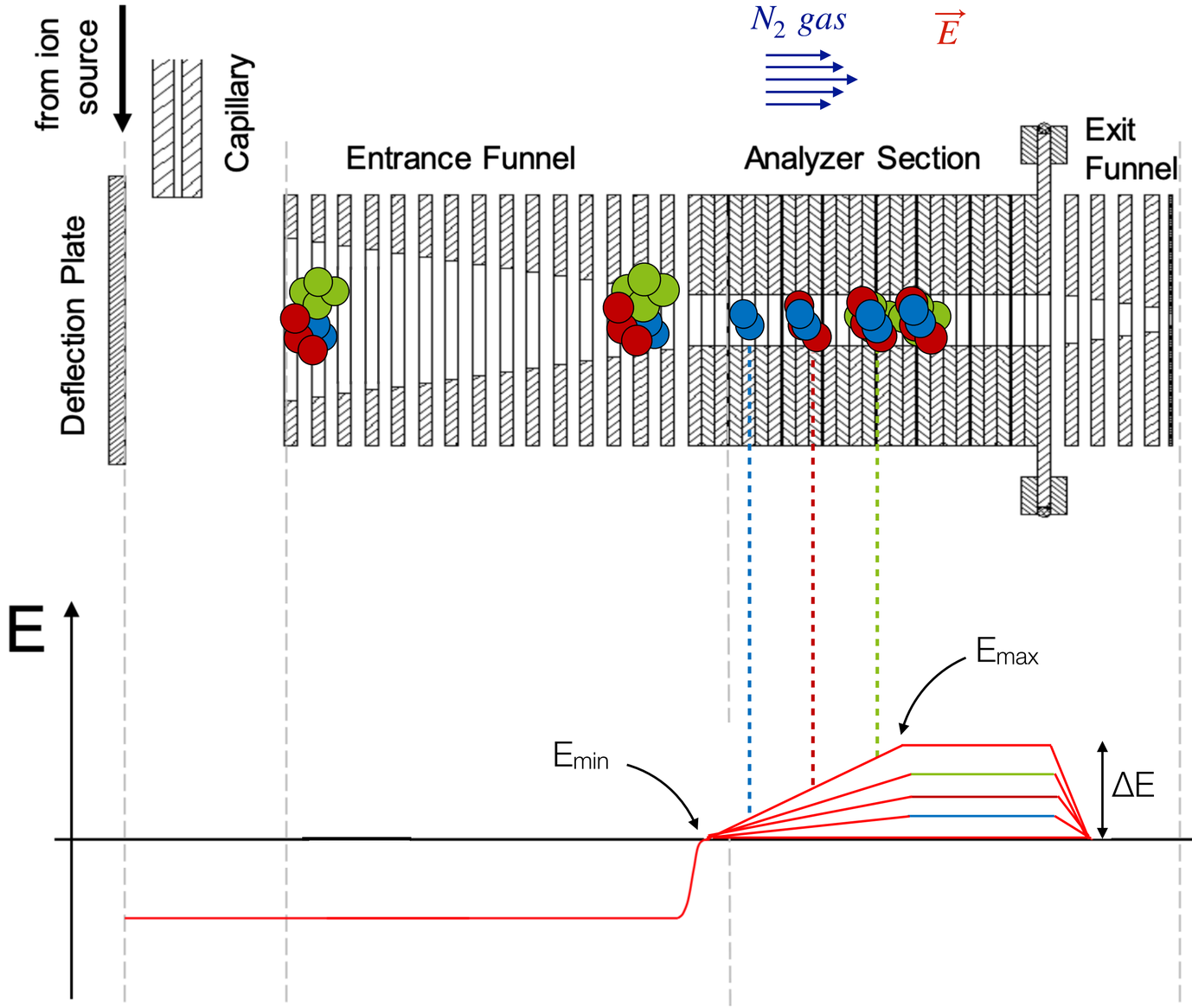
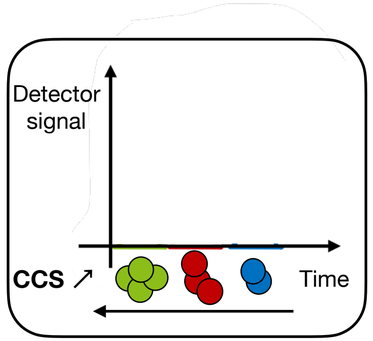
TIMS





1) Accumulation
2) Trapping/Separation
3) Elution

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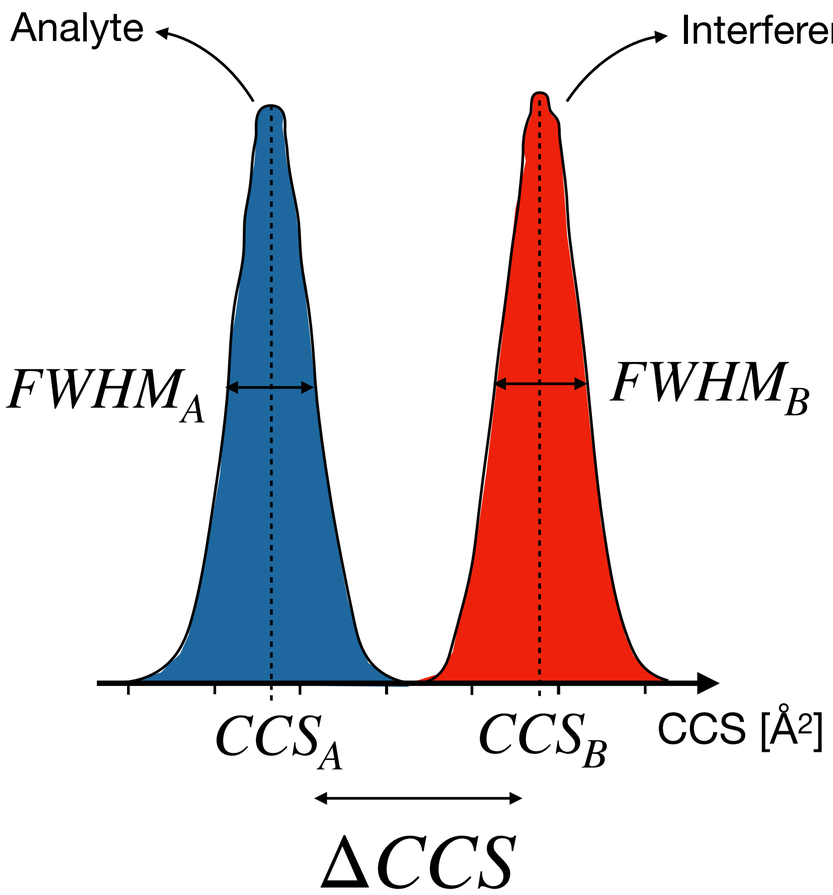
Resolving power in IM

Resolving power

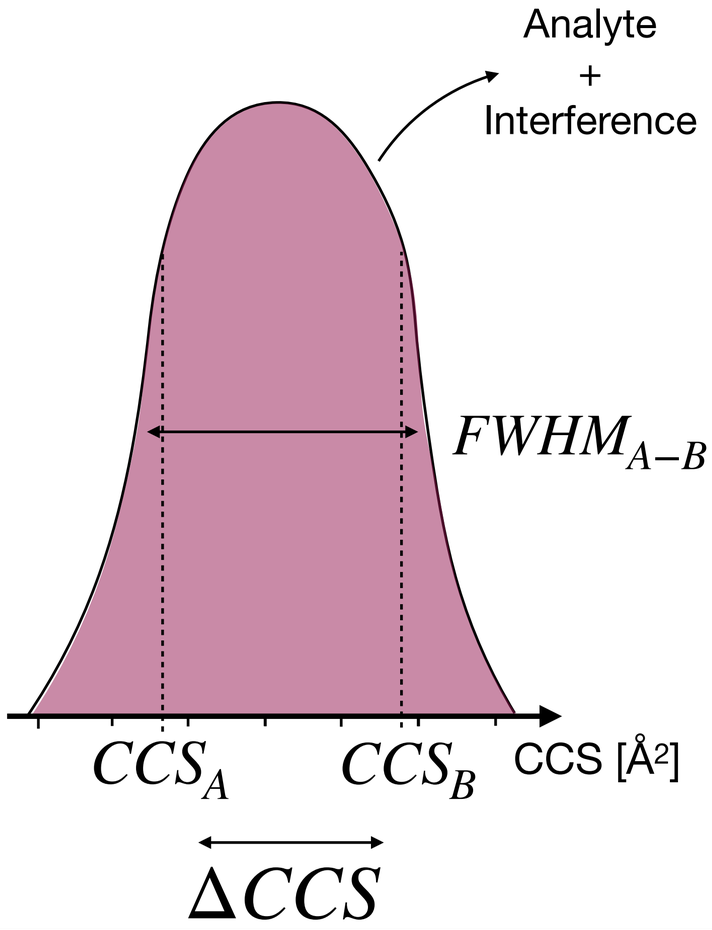
High resolving power



Resolving power

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

Low resolving power



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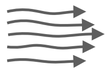
R_p in TIMS

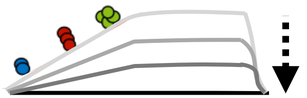
$$R_P \propto \frac{v_g}{\sqrt[4]{\beta}}$$

How to increase R_p?

Increase v_g
⇒ Pratical limit

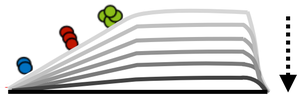


Decrease $\beta \propto \frac{Ion\ mobility\ range}{Ramp\ time}$

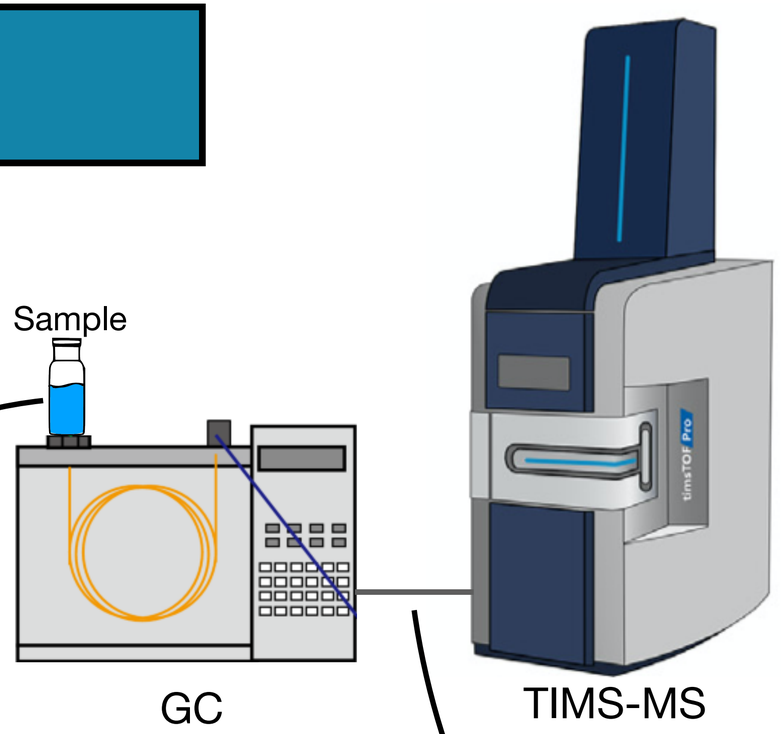


Decrease ion mobility range

Increase ramp time

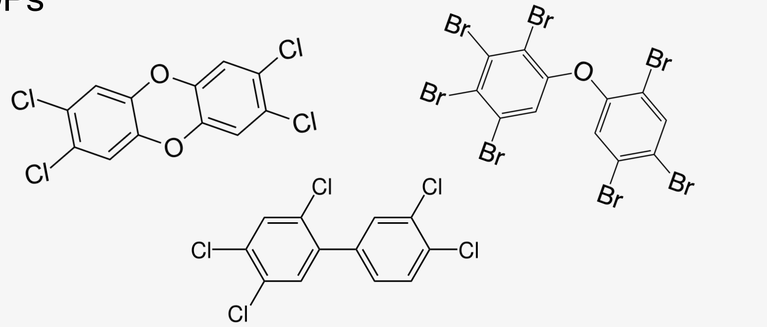


β in GC-TIMS



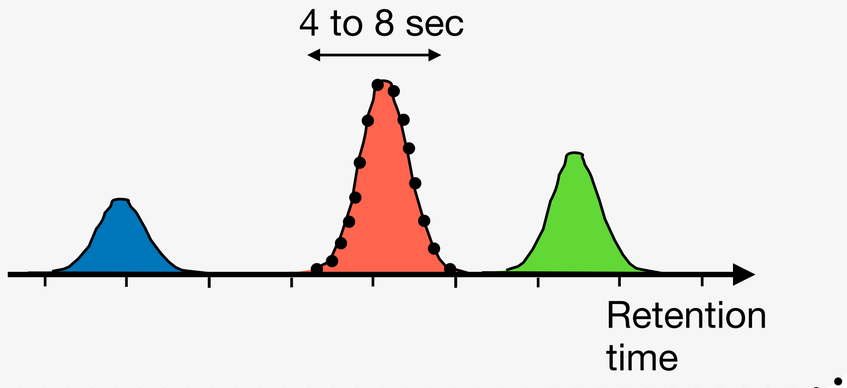
Limitation 1: Ion mobility range

⇒ **Large** ion mobility range to screen many classes of POPs



Limitation 2: Ramp time

⇒ 250 to 350 ms max to have good chromatographic peak sampling (≥10 spectra/peak)



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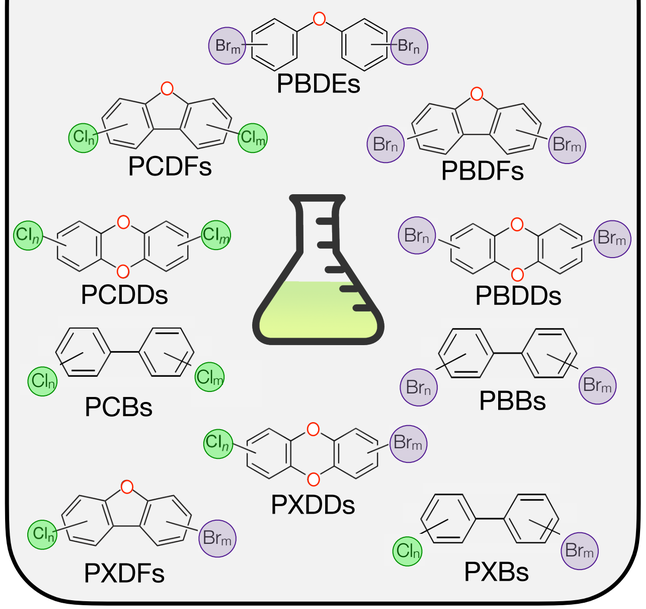
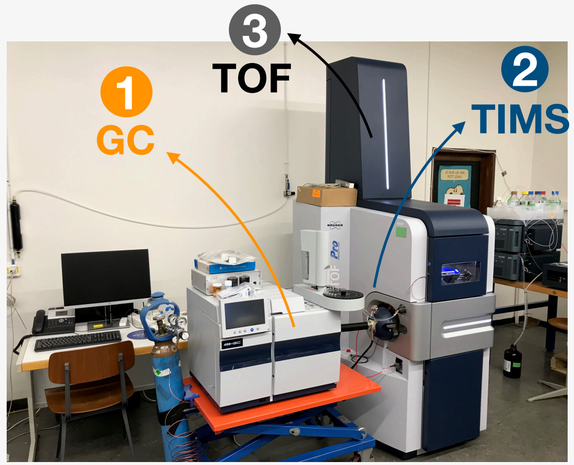
β in GC-TIMS

Mixture of 174 POP standards



GC-TIMS-MS analysis



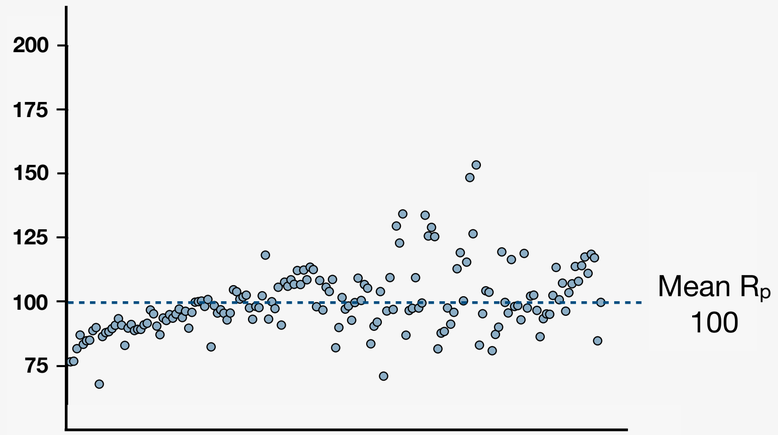
TIMS parameters

Ramp time:
350 ms

Ion mobility range:
1.00 - 1.67 K_0 (0.6 - 1.0 $1/K_0$)

$$\beta_v = 145\ V/s$$

Resolving power



Can we still improve the resolving power?!

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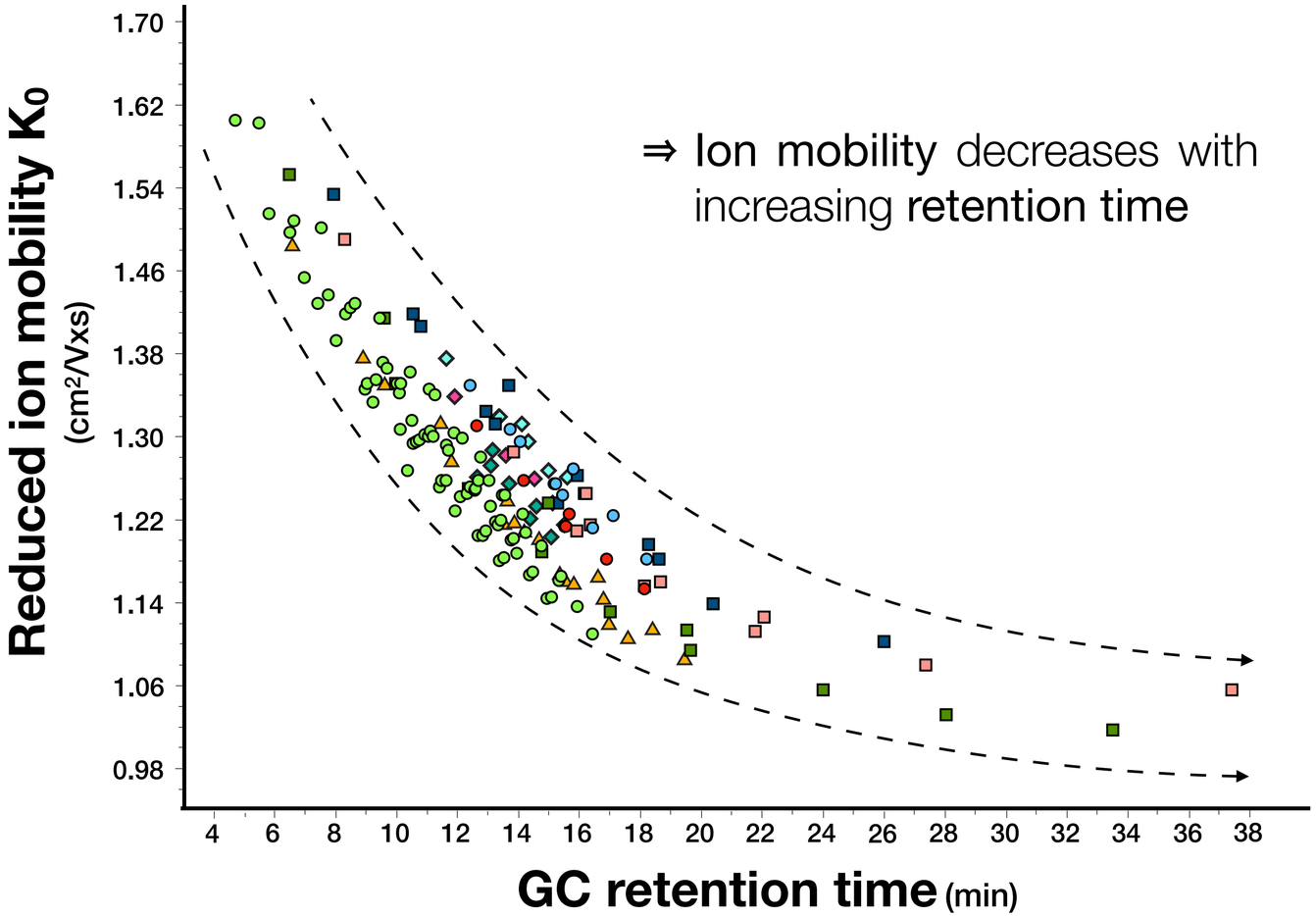
SWIM

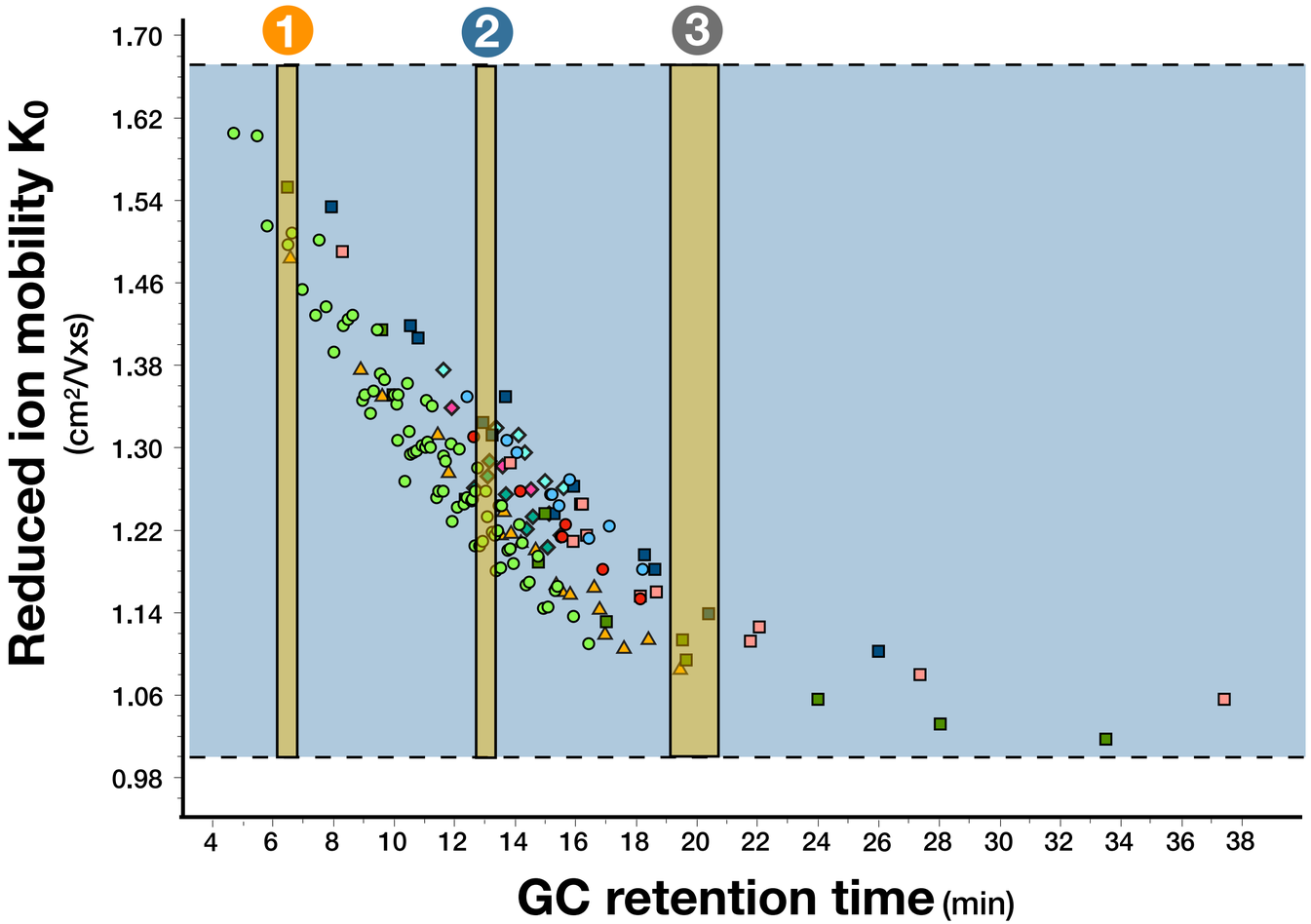
Sliding Windows in Ion Mobility

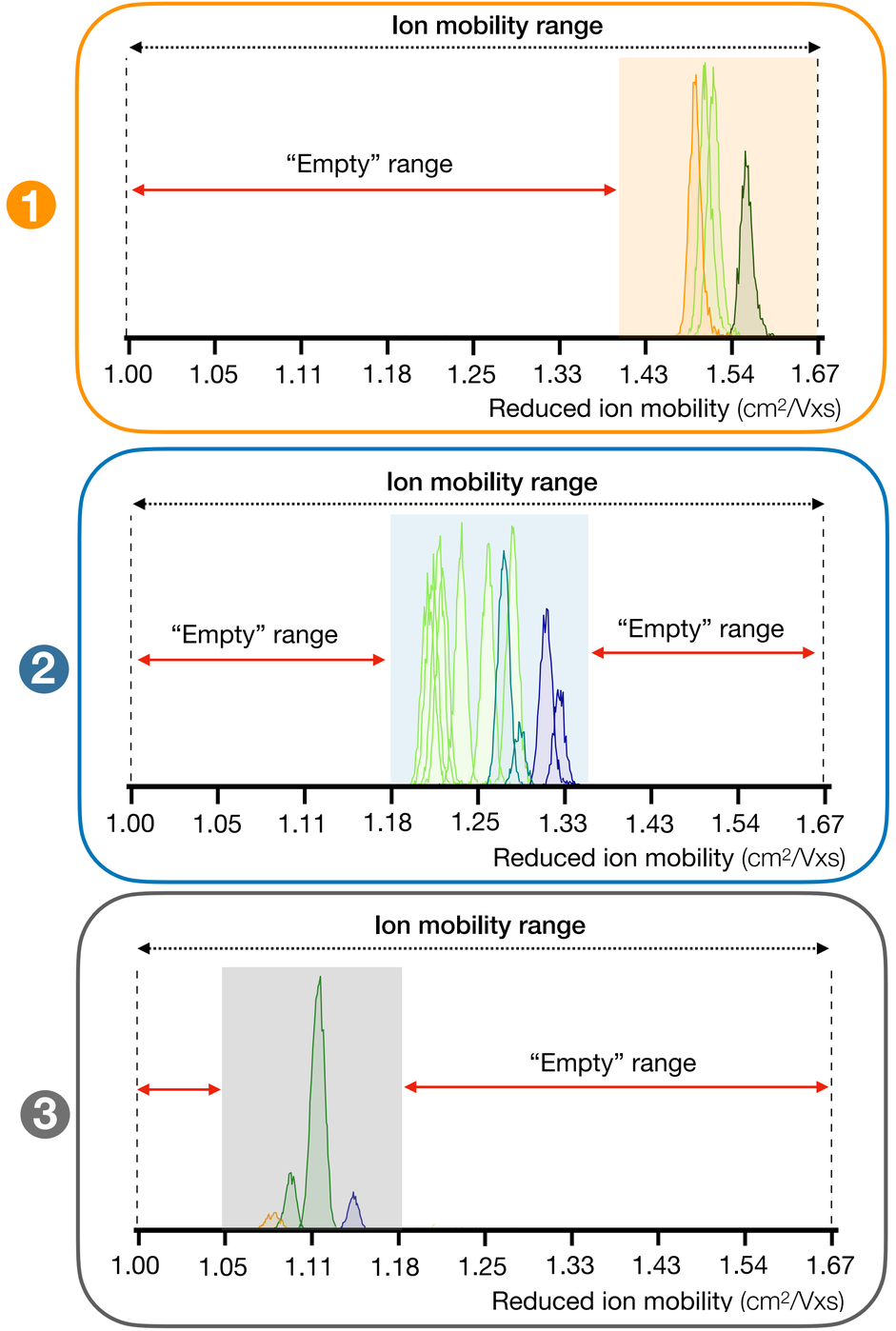
Standard TIMS mode



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

Standard TIMS mode





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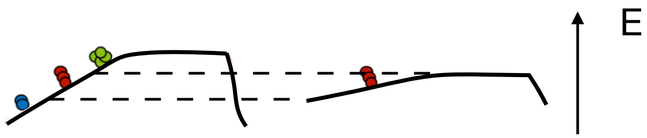
Standard TIMS mode

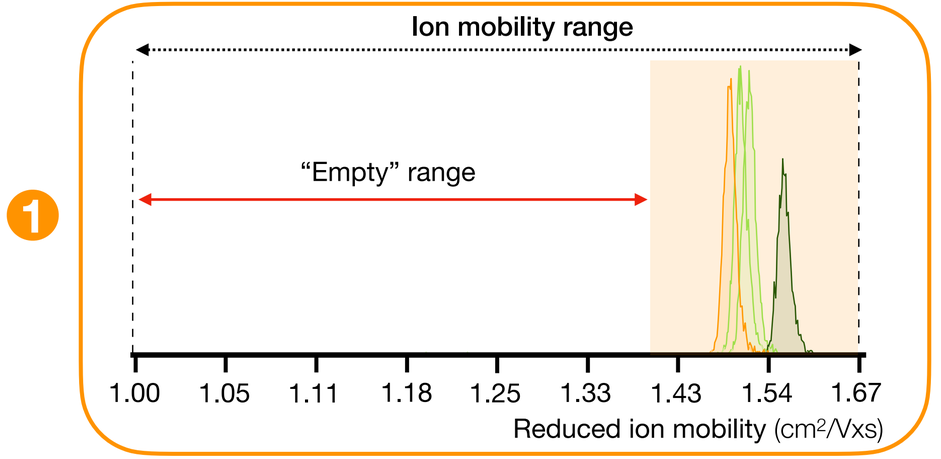
→ Analytical effort is spent focusing on IM ranges that are not relevants

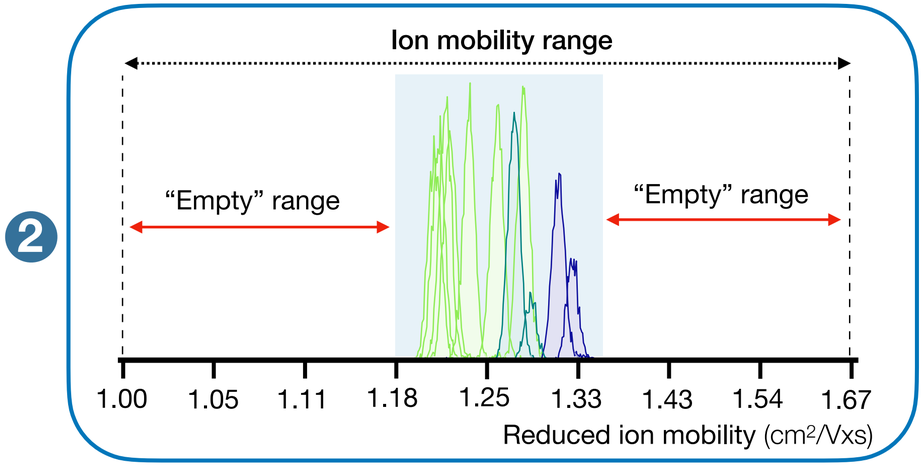
⇒ Limited resolving power!

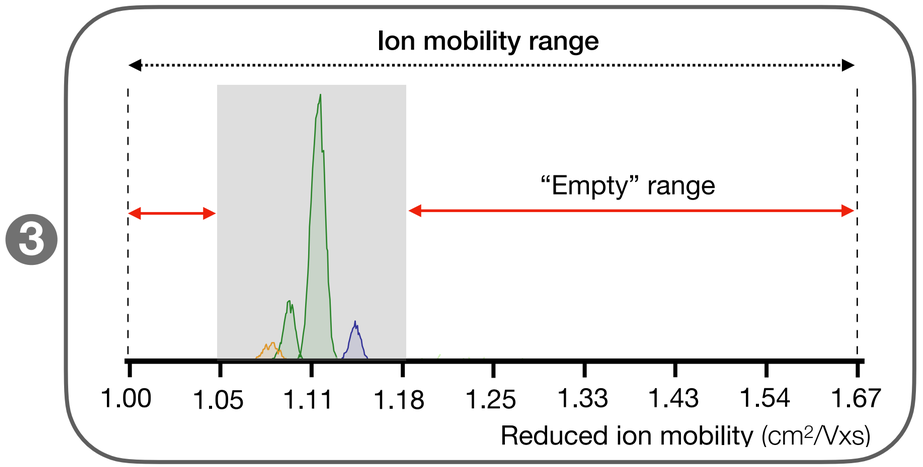
But…

In TIMS, the profile of the electric field gradient can be easily tuned to focus on a given IM range

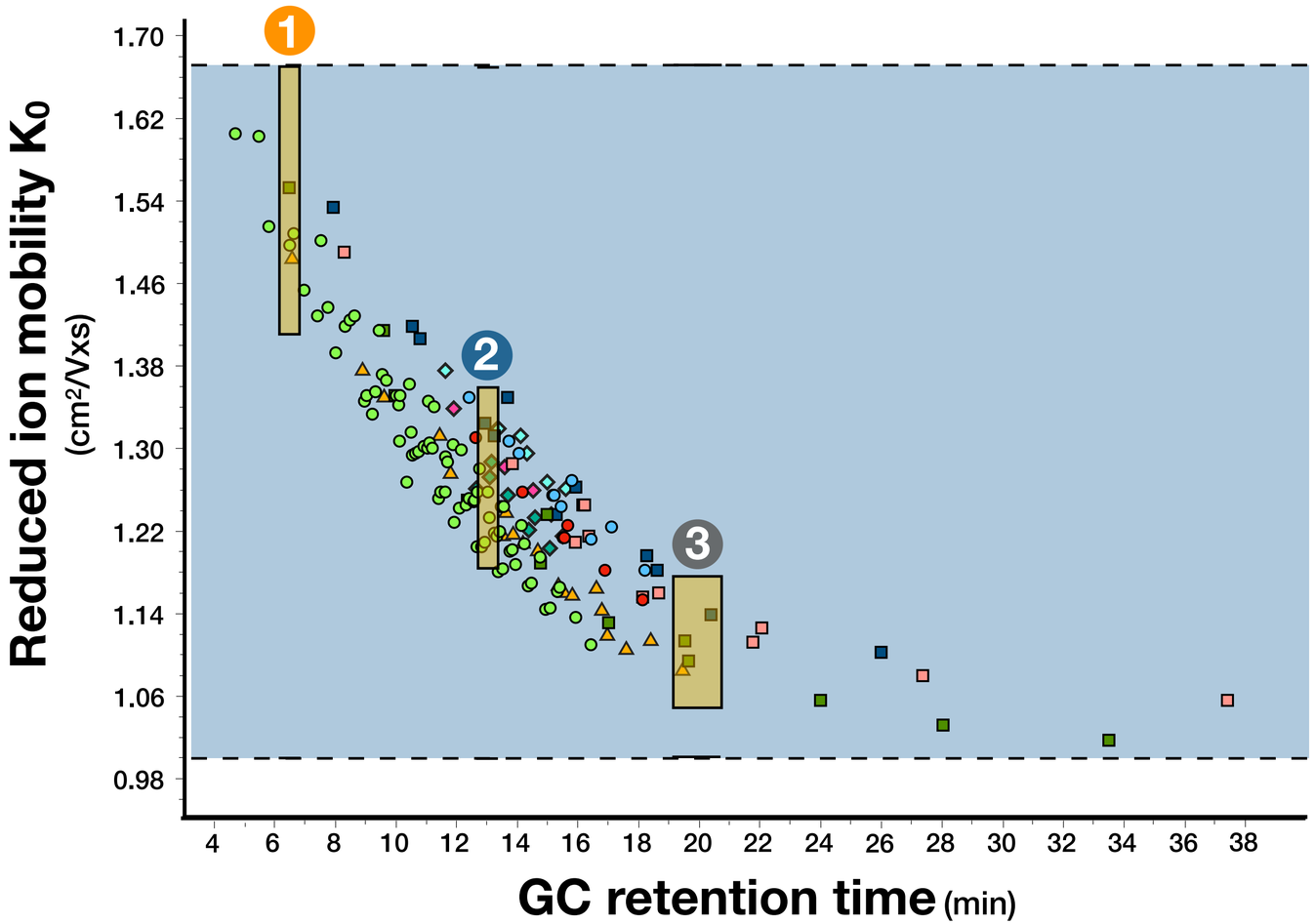


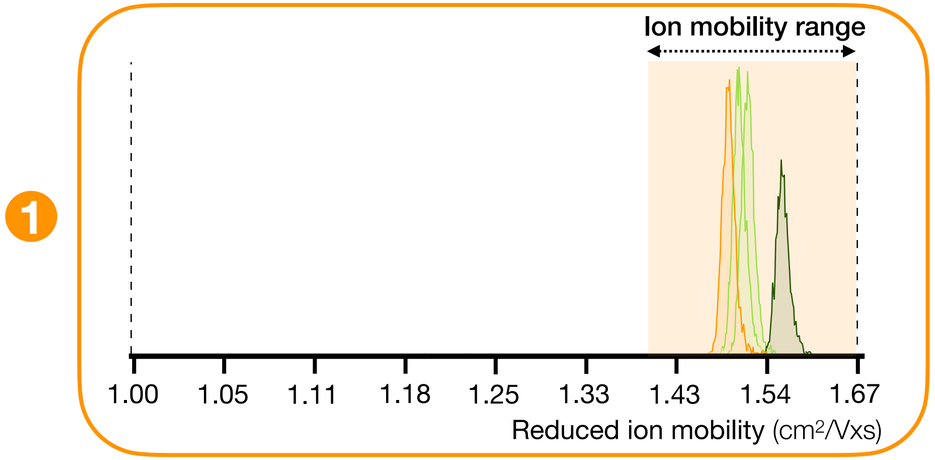


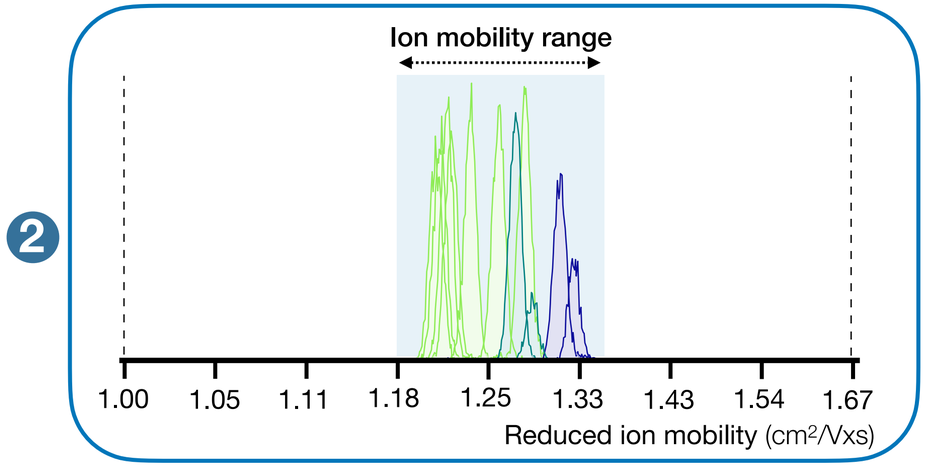


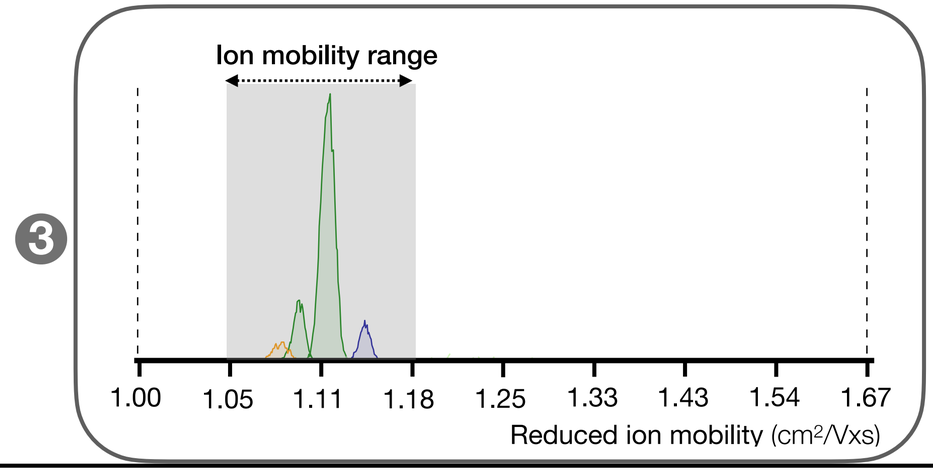


Standard TIMS mode









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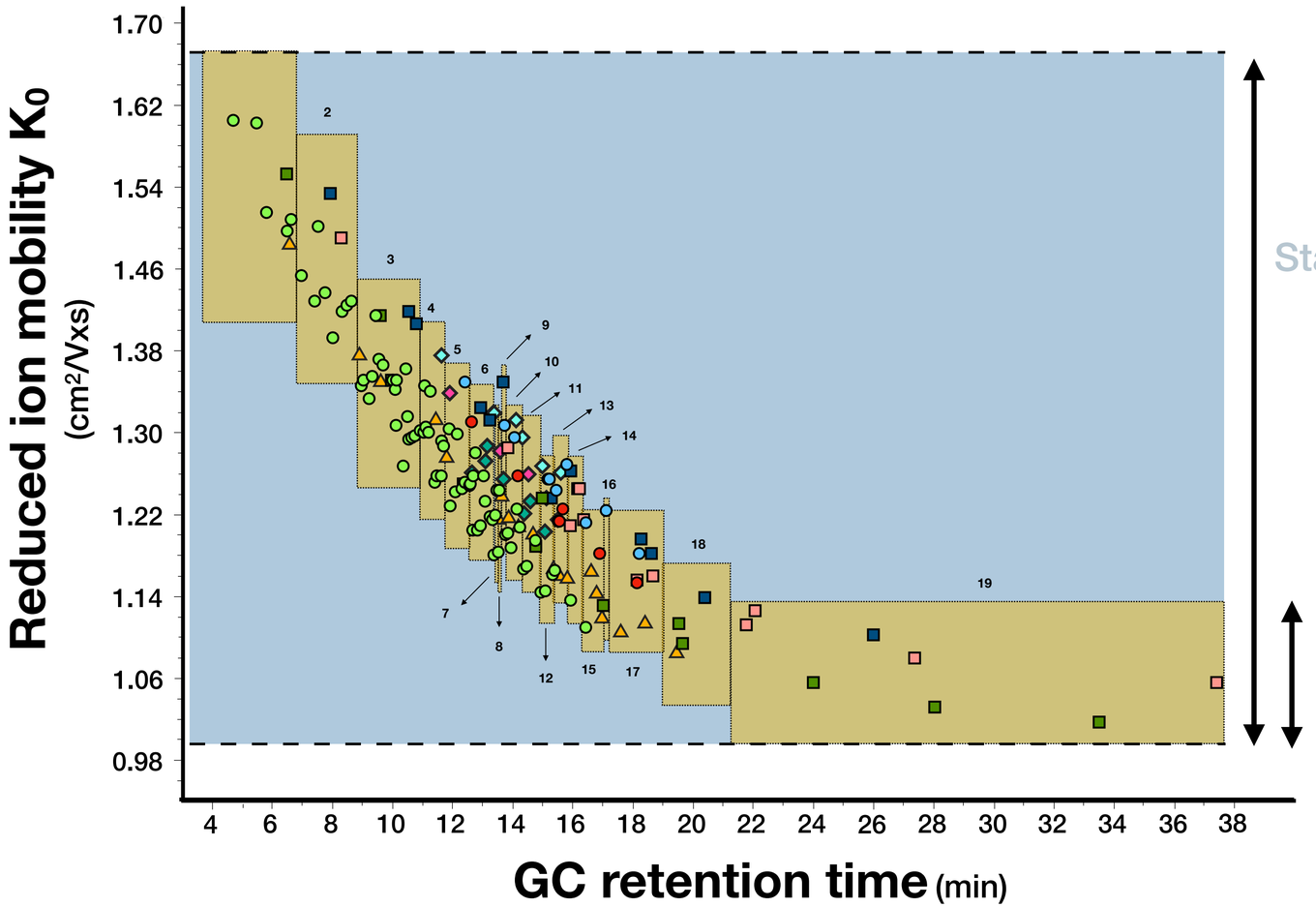
SWIM TIMS mode



Standard mode

SWIM mode
⇒ β_V 40 V/s

~ 4x decrease

Sliding
Windows
Ion
Mobility

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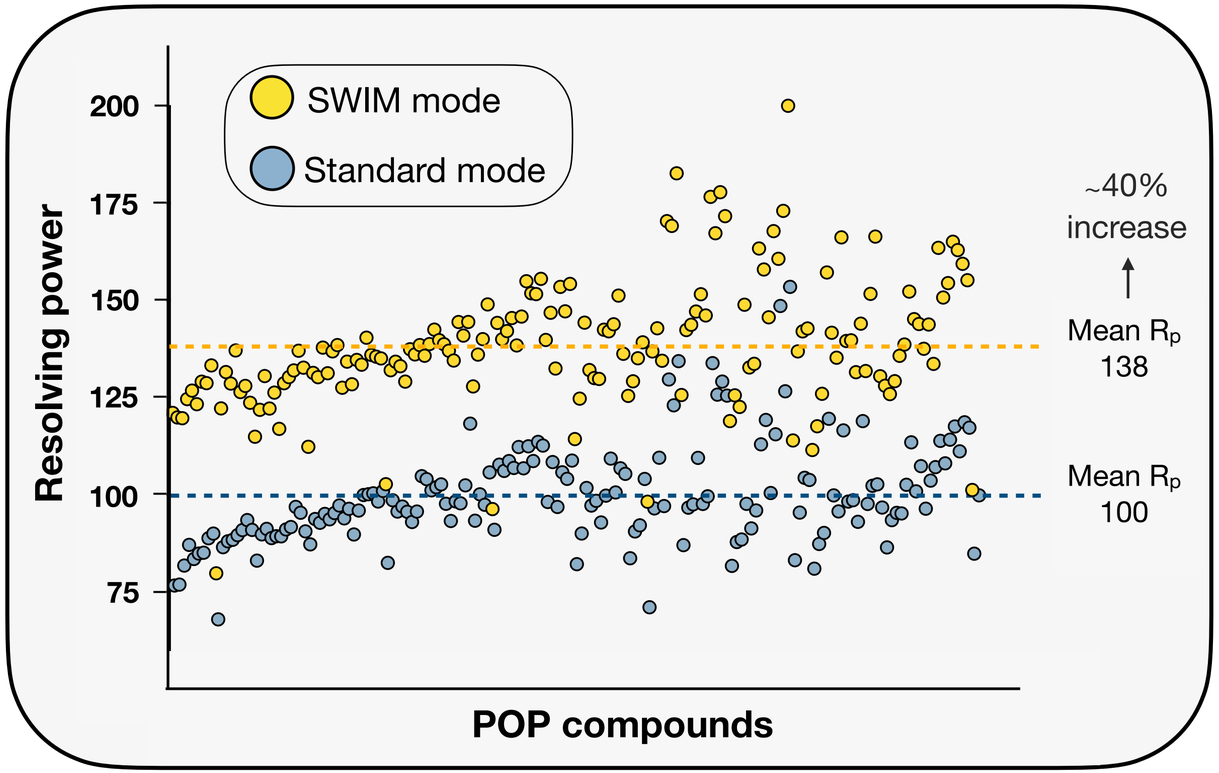
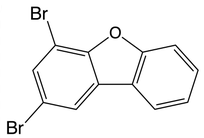
R_p improvement

Expected:

$$\frac{R_{p(SWIM)}}{R_{p(Standard)}} = \sqrt[4]{\frac{\beta_{v(Standard)}}{\beta_{v(SWIM)}}} = \sqrt[4]{\frac{145}{40}} = 1.38 \longrightarrow \text{~40\% increase}$$

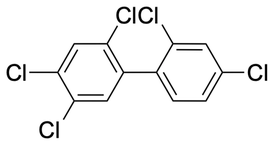


Selectivity improvement



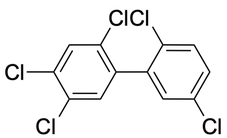
2,4-DiBDF

m/z 325.87**60**



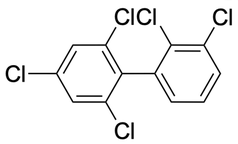
PeCB 90

m/z 325.87**99**



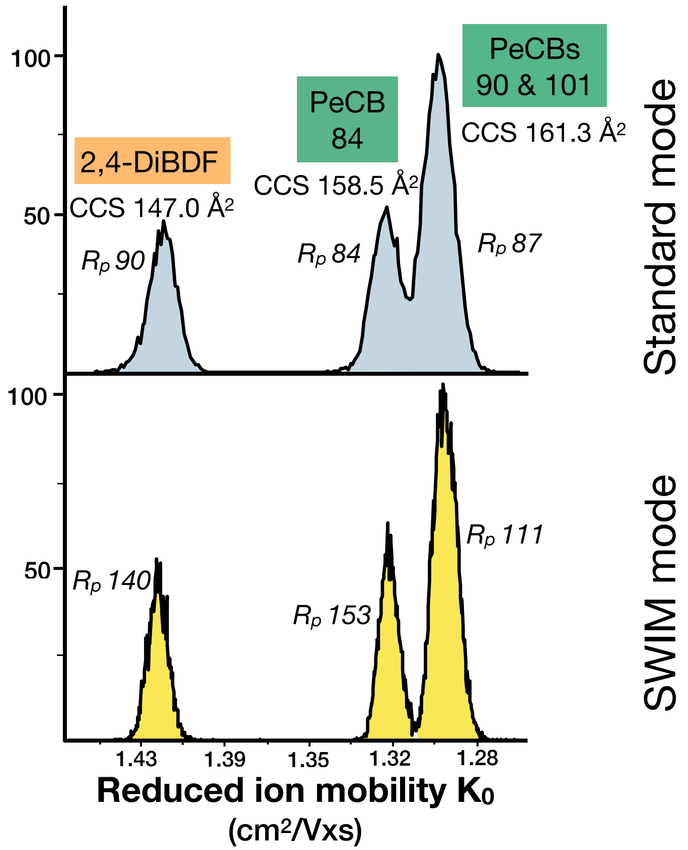
PeCB 101

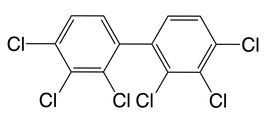
m/z 325.87**99**



PeCB 84

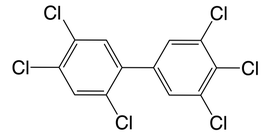
m/z 325.87**99**





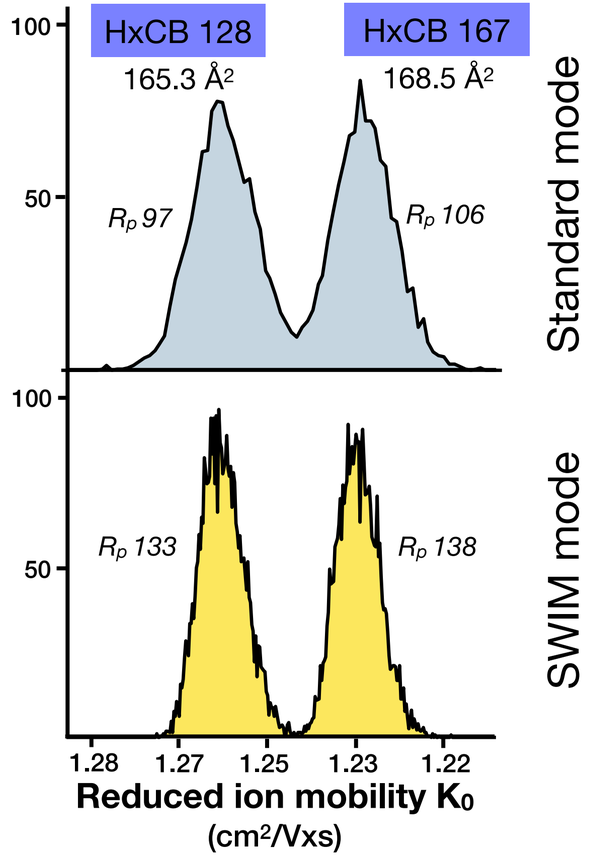
HxCB 128

m/z 359.8410



HxCB 167

m/z 359.8410



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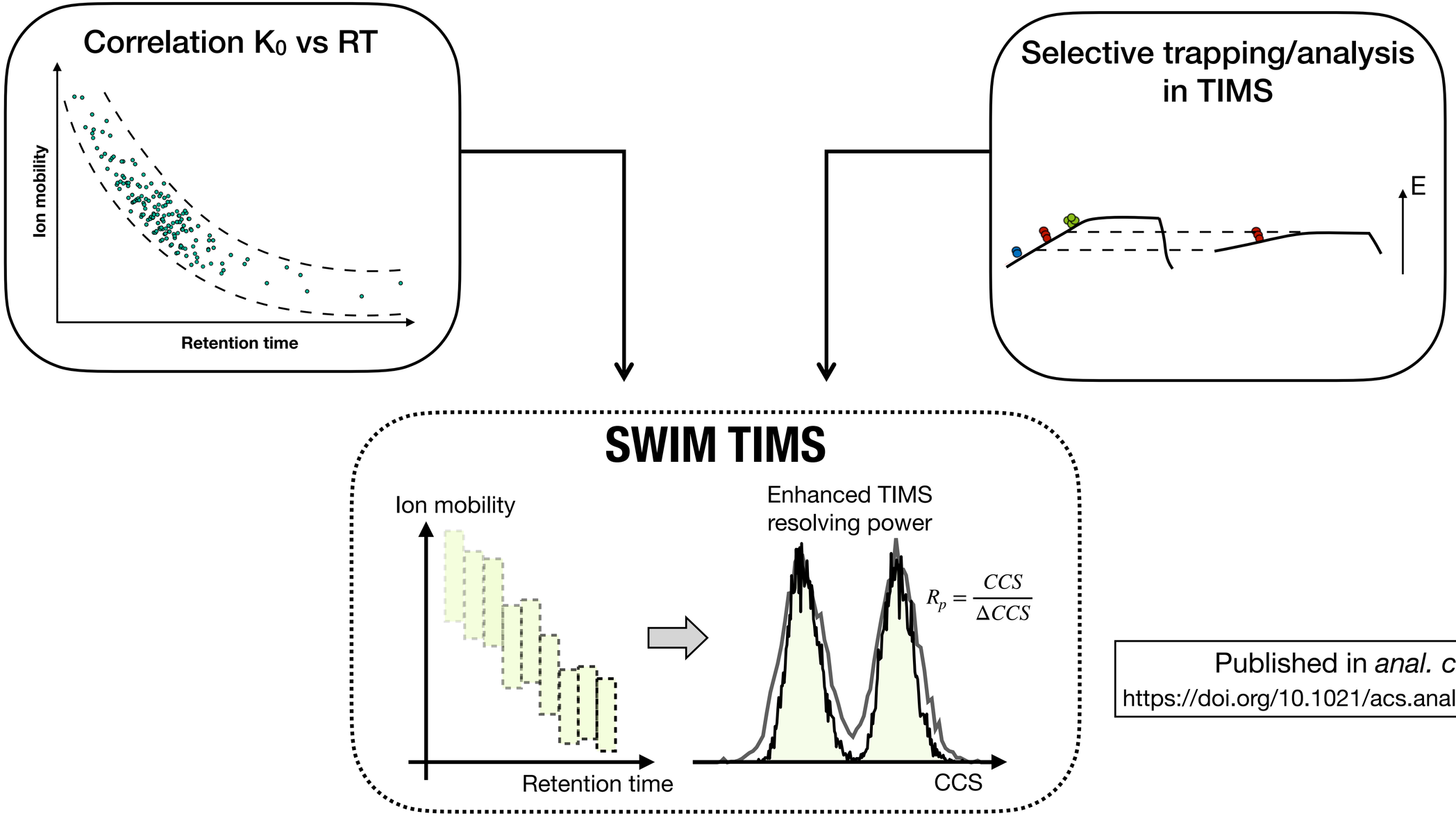
Conclusion

Summary



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SPECTROMETRY

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

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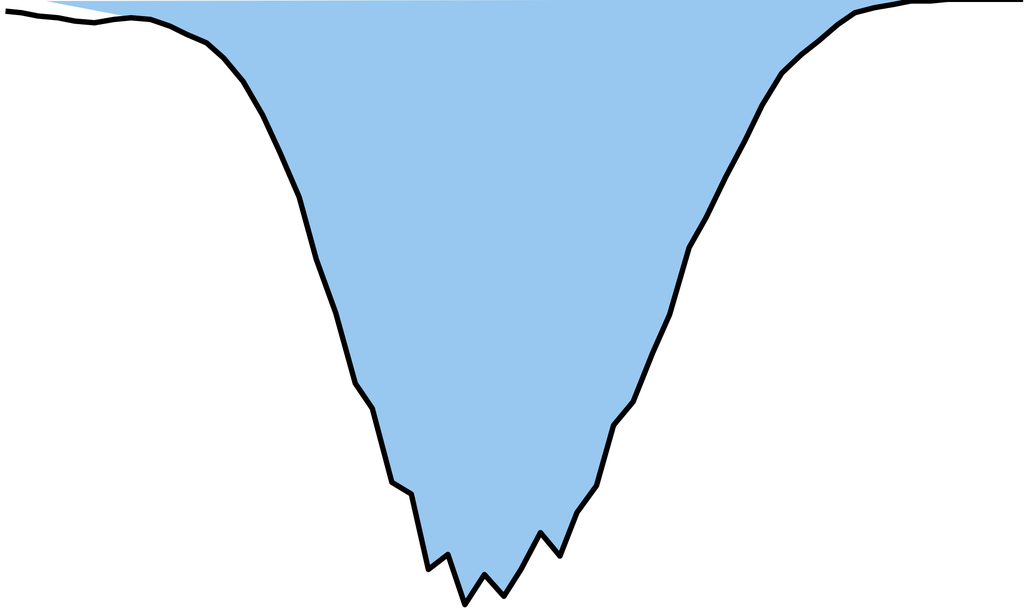
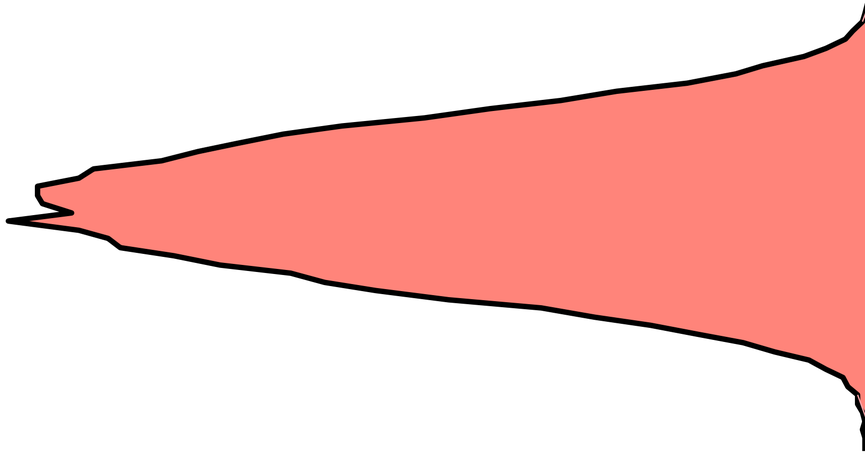
fnrs FREEDOM TO RESEARCH





Thank you