

# Evaluation of GC-Orbitrap for urine volatolome investigation

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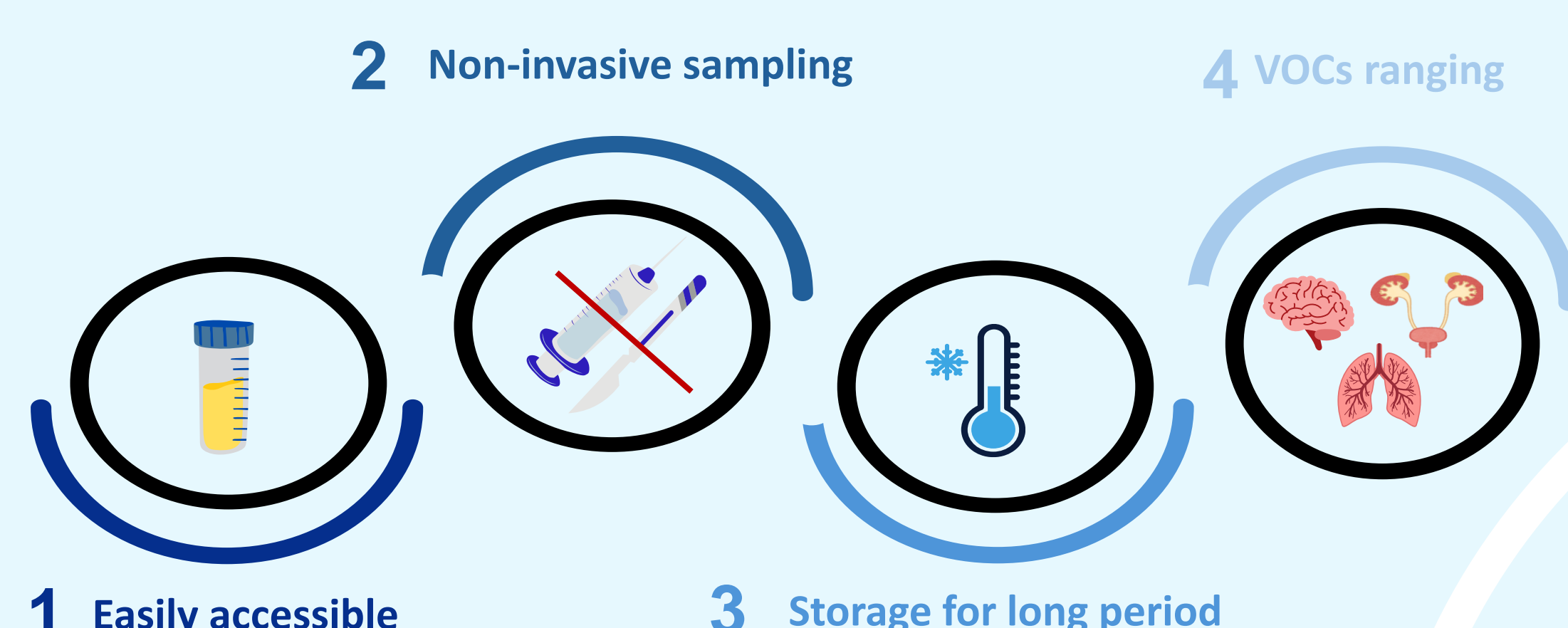
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## I- Introduction

Volatolomics is a research field focused on analyzing volatile organic compounds (VOCs) emitted by biological systems. These compounds reflect metabolic states and offer non-invasive diagnostic possibilities for diseases [1]. However, volatolome investigation relies on an untargeted analysis strategy. Therefore, it requires optimization of operating conditions to detect a wide variety of compounds and limit the instrumentation variability.

🎯 This study aims to optimize various parameters for the detection of numerous compounds and to assess the variability of the GC-Orbitrap analyzer.

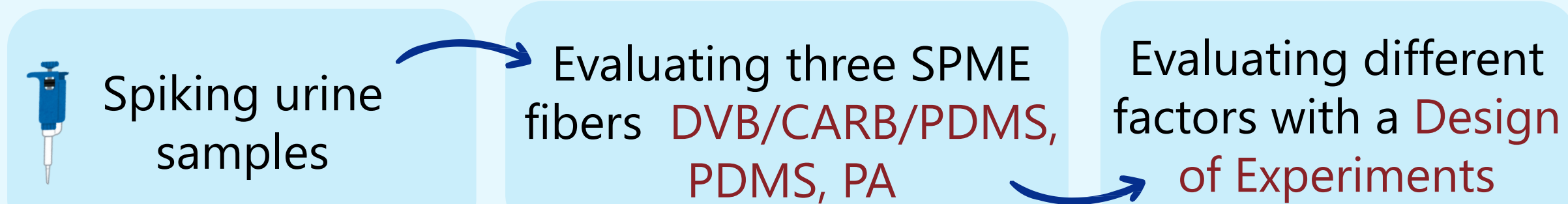
### Urine, A Matrix of interest



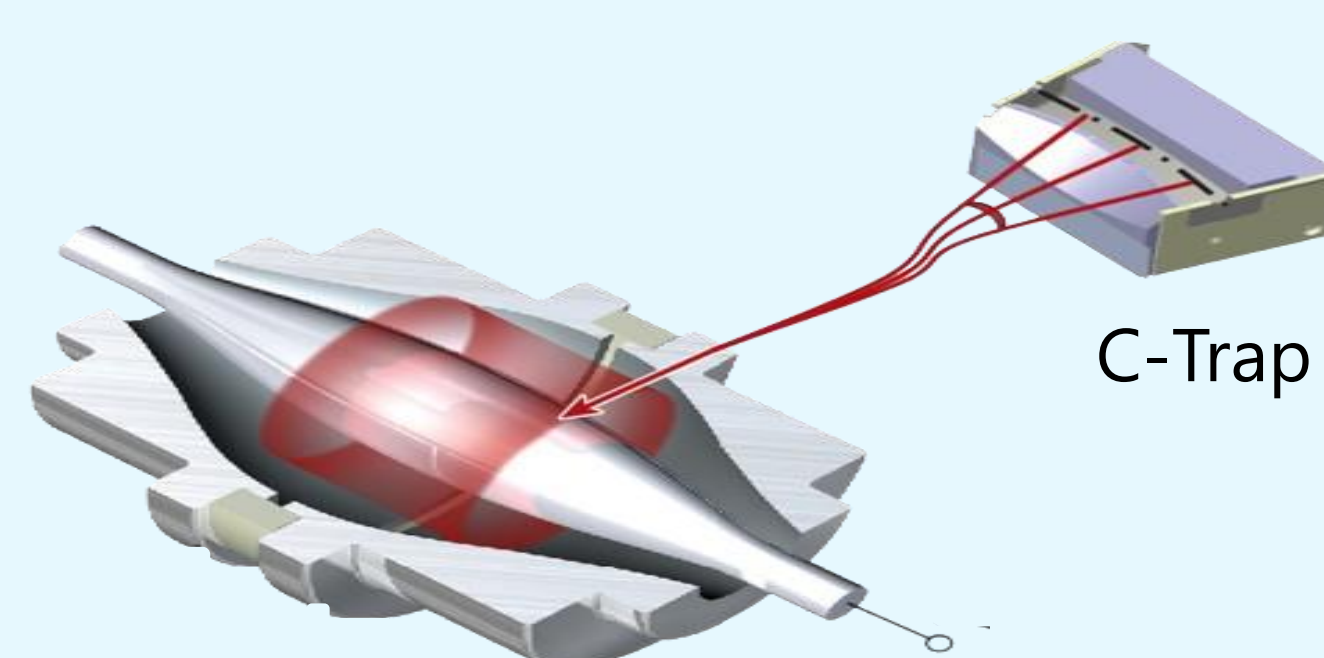
## II- Strategy

### » Optimization

Sampling conditions were optimized using a GC-QMS (Scion).

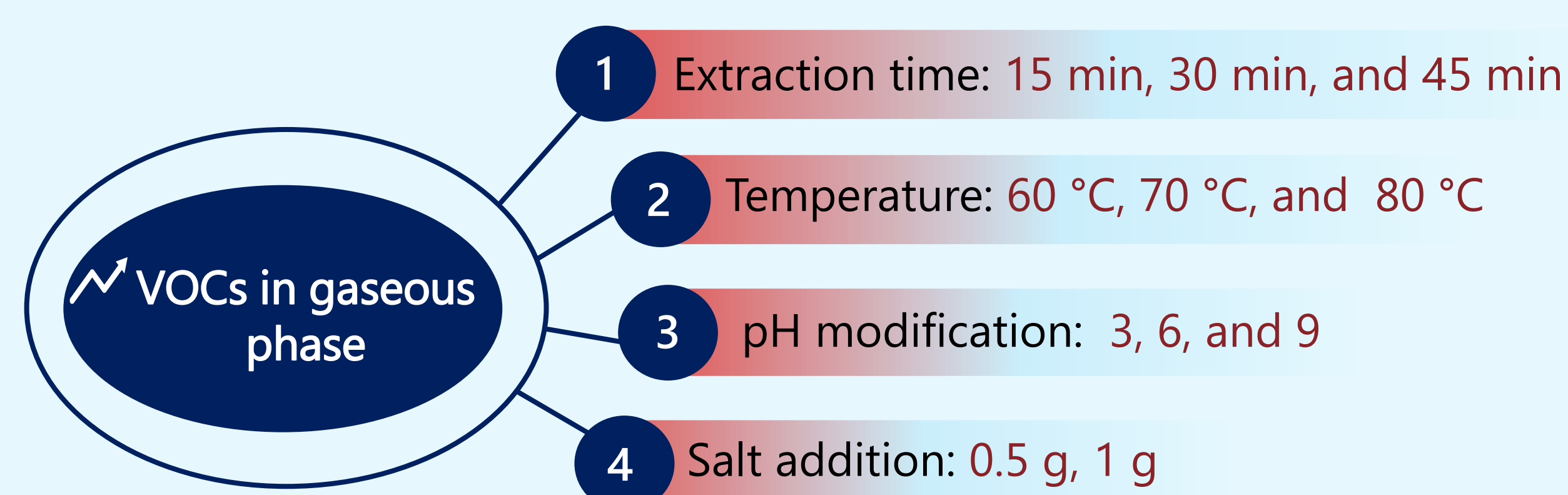


### Orbitrap analyzer



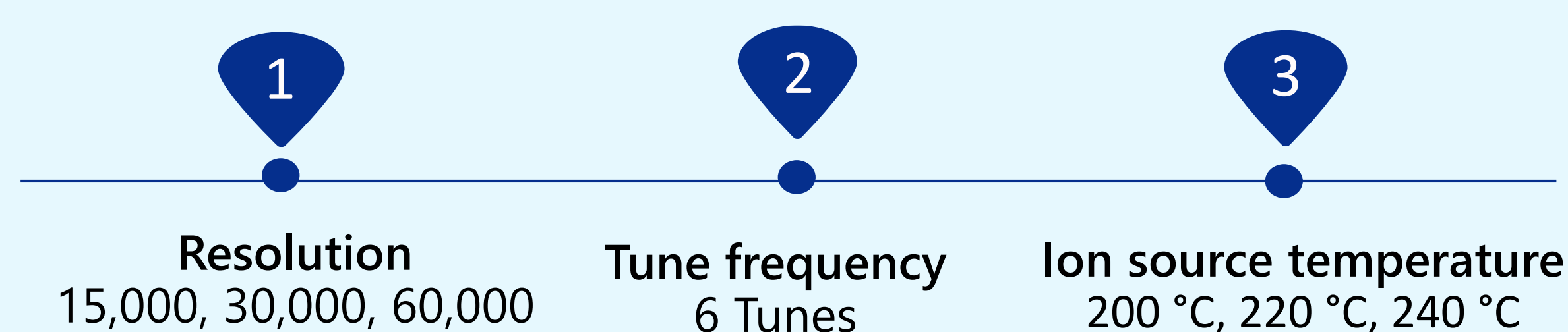
**AGC target :** The number of ions in the C-trap before injecting : **1 millions ions**

**Max inject time :** The maximum time that ions are allowed to accumulate in the C-trap [2]  
**set at 5 ms**



### » Variability study: GC-Orbitrap

A mixture of 14 compounds of different chemical classes was analyzed, and peak areas of the most intense ions were taken into account for each compound.

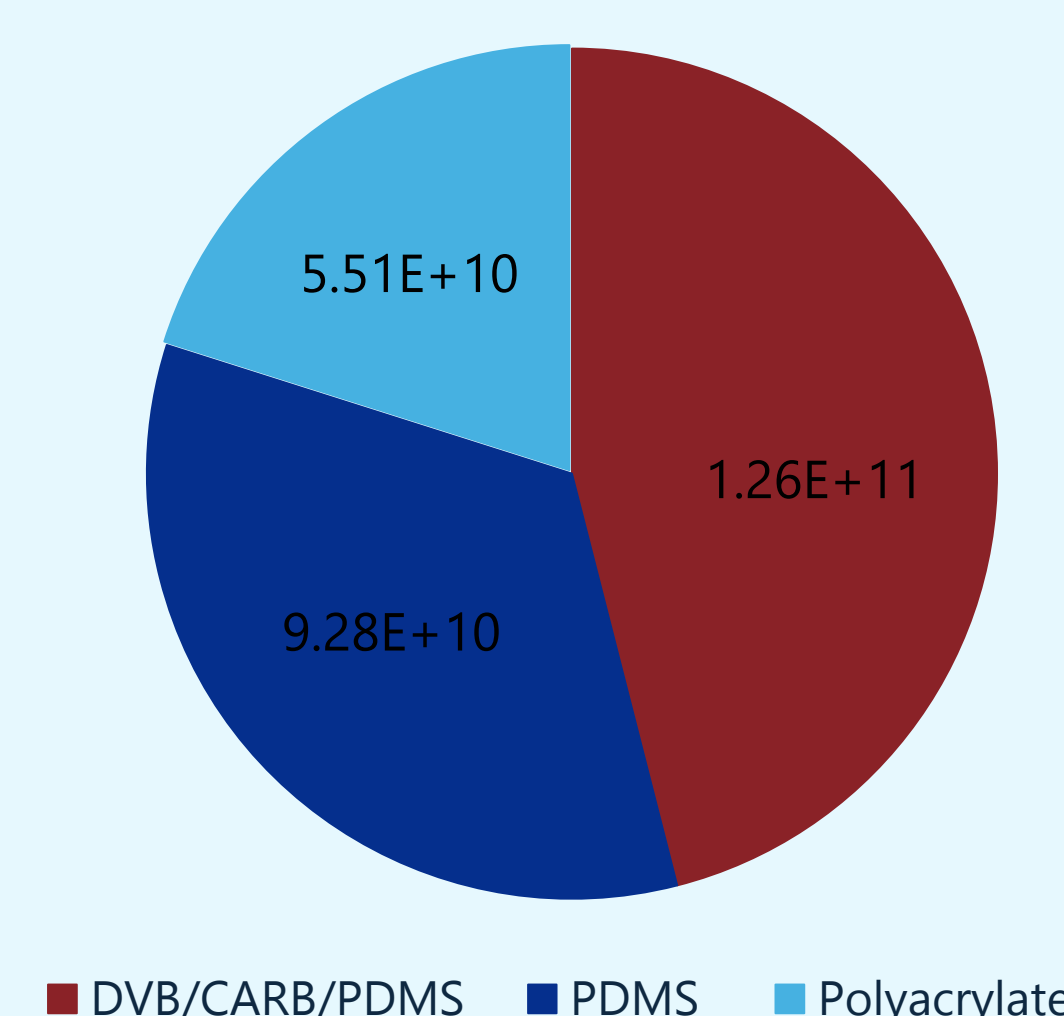


## III- Results

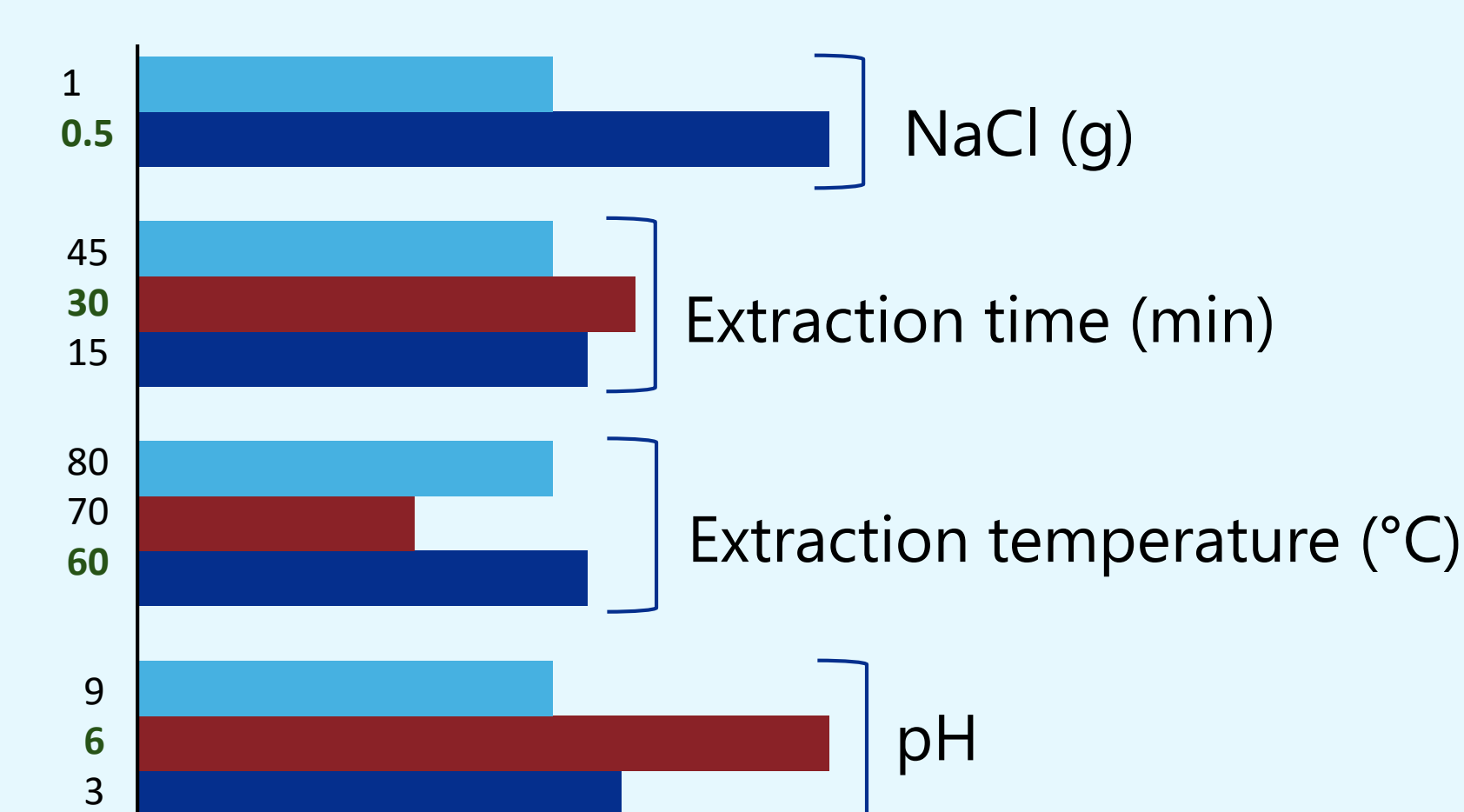
### » Optimization

Sum of areas were used to evaluate the effects.

#### Choice of coating fiber



#### Total effect plot



- ✓ The most suitable fiber is **DVB/CARB/PDMS**.
- ✓ The optimal conditions obtained with software Azurad are pH 6, extraction T°C. 60°C, extraction time 30 min, and NaCl 0.5g.

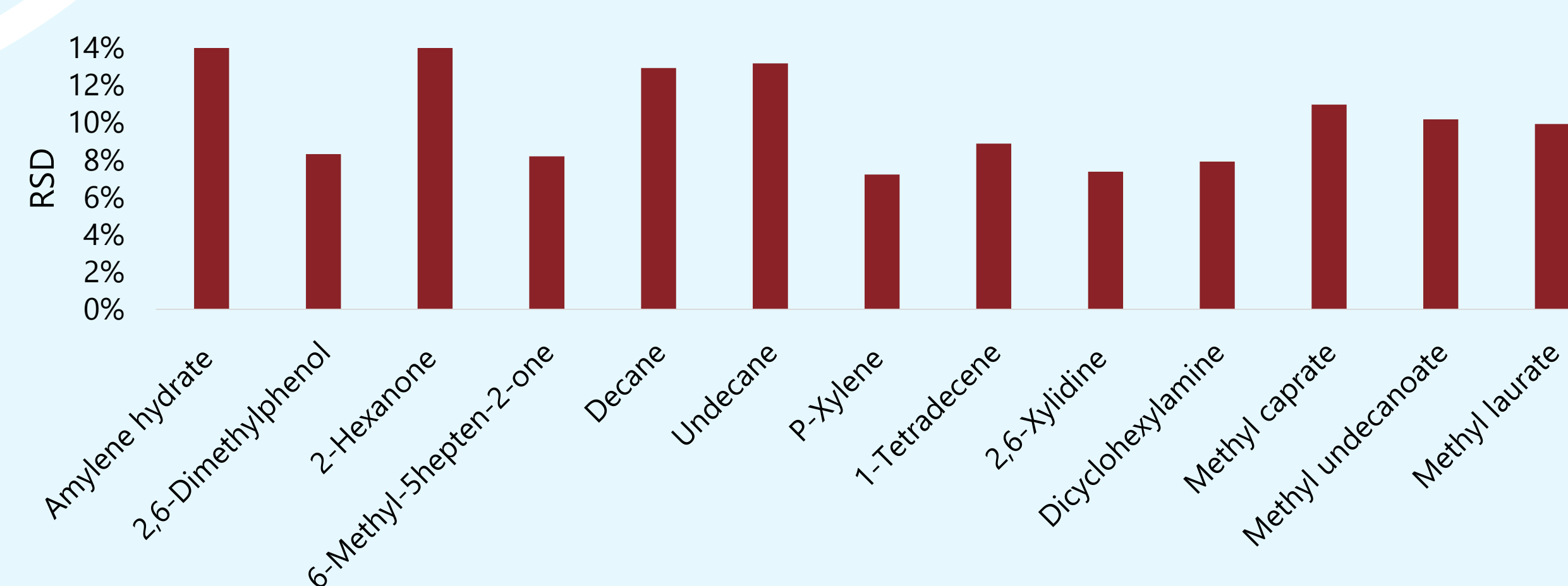
### » Variability

#### 1- Resolution

Resolution	Frequency (Hz)
15,000	23.26
30,000	14.38
60,000	7.42

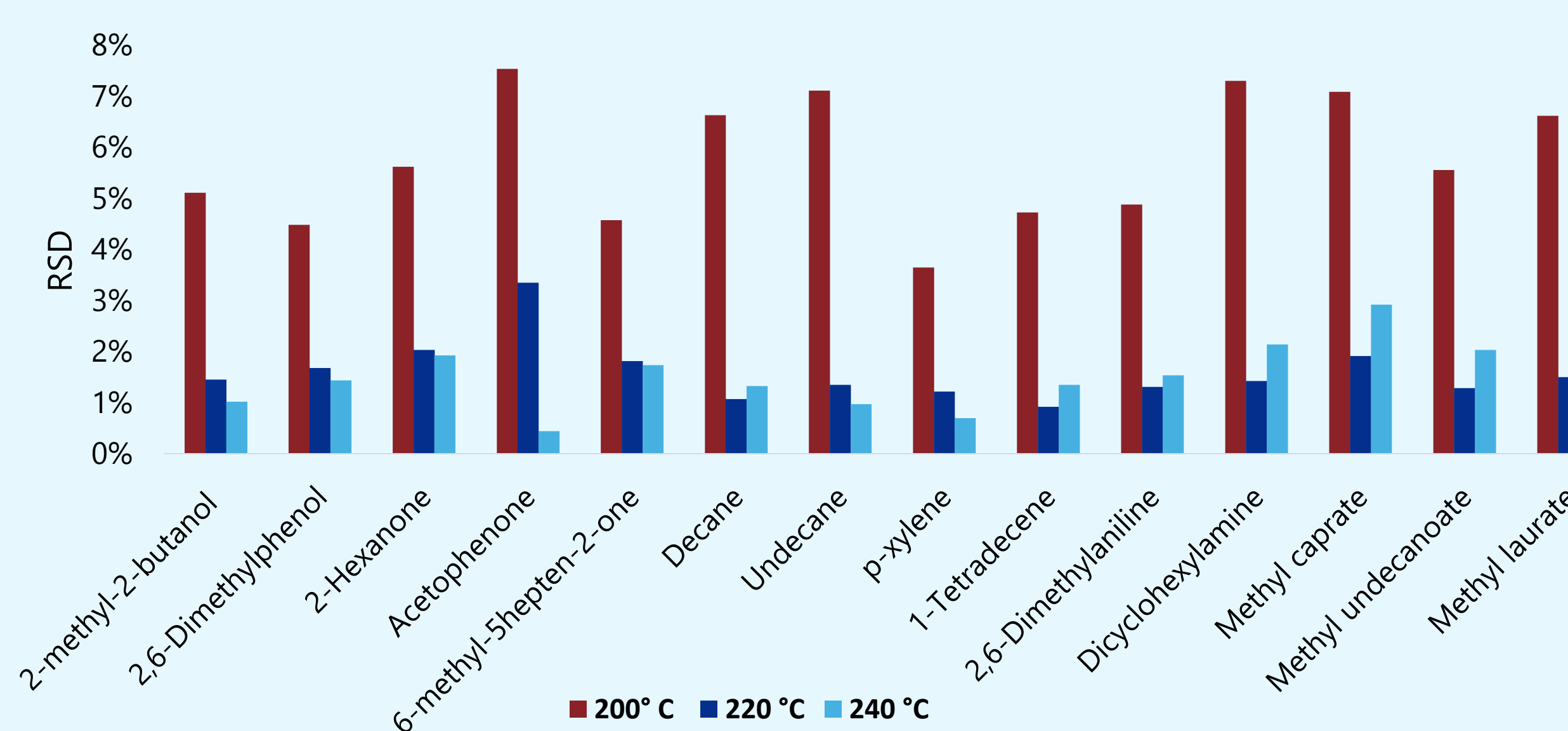
The resolution has a significant impact on the acquisition rate.

#### 2-Tune frequency



- ✓ The variability of the areas when testing 6 tunes is at most 15 %, which is acceptable.

#### 1- Ion source temperature



- ✓ Ion source temperature affects area variability, with less significant impact at 240 °C.

## IV- Conclusion/ Perspectives

- 🎯 The optimal parameters for urine analysis were obtained, and the variability study shows that the ion source temperature affects fragmentation (less significant at 240 °C), area variability is not important while performing different tunes, and resolution impacts the acquisition rate.
- 🔭 Move on to comprehensive two-dimensional gas chromatography (GC×GC-Orbitrap), and analysis of patient urine samples to determine biomarkers of prostate cancer.

## References

- [1] Hu, W.; Wu, W.; Jian, Y.; Haick, H.; Zhang, G.; Qian, Y.; Yuan, M.; Yao, M. Volatolomics in Healthcare and Its Advanced Detection Technology. *Nano Res.* 2022, *15* (9), 8185–8213.
- [2] Eliuk, S. M.; Makarov, A. A. Evolution of Orbitrap Mass Spectrometry Instrumentation. *Annu. Rev. Anal. Chem.* 2015, *8*, 61–80.