User-friendly method for GC×GC optimization

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Conclusions

The **Orthogonality Index** (OI) calculation allows GC×GC user to have a **quantitative evaluation** of their column sets and to classify those.

Based on this tool, four different types of orthogonality where define: the **Normal**, the **Reverse**, the **Hybrid** and the **Transpose** orthogonality. This classification is based on the separation pattern obtain on the 2D space.

This method in addition to other numerical parameters can help people to choose the best column set and to optimize their GC×GC methods.

Context

Introduction

Why do we use GC×GC for complex samples analysis?

There are plenty of reasons but the biggest one is the **additional dimension of separation**.

Challenge

GC×GC is a really power full tool. Unfortunately, the optimization step is not obvious due to the huge number of parameters that can be change.

The final method is, most of the time, the best compromise.

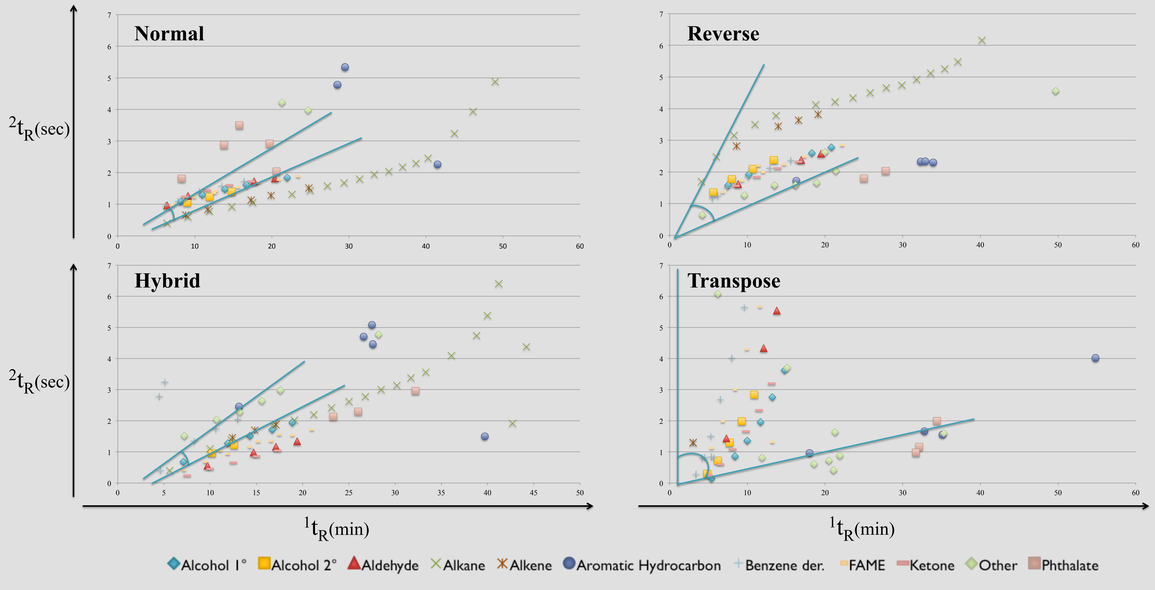

Figure 1: Century mix injections on the different kind of orthogonality combination and visualization of the OI.
N.B: All the injections were done in the same GC condition.

Results & Discussion

Basis of this study: The Century Mix

The descendant of the Phillip mix!

- Mix of homologous series of different chemical families
- Around 120 compounds
- Design to be an evaluation tool for GC×GC users

Classification method

There are more and more columns available on the market. With the new type of phases (e.g. liquid ionic), the range of polarity is constantly growing.

➔ An universal classification method should help people to find the best combination!

Going back to the mathematical definition of the Orthogonality

Orthogonality Index: Measure of the **angle** between C6-C10 line in the **alkane family** and the C6-C10 line in the **aromatic hydrocarbon family**.

➔4 different kind of orthogonality classifications:

Normale Orthogonality: Non-polar – Semi-polar

Reverse Orthogonality: Semi-polar – Non-polar

Hybrid Orthogonality: Semi-polar – Semi-polar

Transpose Orthogonality: Extremely-polar – Non-polar

Orthogonality Index values		
	OI	**SD**
Normal Orthogonality	2,53	0,17
Reverse Orthogonality	-13,12	0,12
Hybrid Orthogonality	3,38	0,18
Transpose Orthogonality	-87,23	0,02

Table 1: OI values calculated on triplicate injections

Some interesting observations:

Surprisingly, the Normal orthogonality has a smaller OI than the Hybrid one. The Hybrid combination is not orthogonal based on the strict definition but for some compounds, it offers a better separation than the most used column combination.

The Transpose orthogonality can be really helpful for semi-polar compounds separation but the column choice should probably be less extreme.

There are still plenty of combination to test and certainly plenty of interesting information to find in the future of this research…

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