

## User-friendly method for GC×GC optimization

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Almost 30 years are gone since the first paper about multidimensional GC was published by John B. Phillips<sup>1</sup>. After several years of developing process, Comprehensive Two Dimensional Gas Chromatography systems are in the commercialization step of its live time. During this period, the advantages of GC×GC, regarding to classical D1 system, were clearly demonstrated<sup>2</sup>. However, the new parameters involve in a GC×GC method are still not completely understood and people don't use it at the maximum of its capacity. According to the literature more and more groups are using GC×GC for different kinds of applications. In most of these researches, GC×GC was used for its separation power. Unfortunately, the orthogonality and the column set are most of the time poorly optimized. To help people in this important step, we develop an user-friendly method to choose the best column combination and the best separation parameters for a particular application.

All these developments were based on different mix of standard call the Century mix and the Dimandja mix. These are the descendants of the Phillips mix create in 2003 by J. Dimandja<sup>3</sup>. These mixtures contain homologous series of compounds representing the polarity and the volatility range commonly seen in GC×GC.

This method is based on the Retention Index obtained in a classical GC analysis and projected in the 2D space. Using this projection method, we identified four major types of orthogonality based on the peak dispersion obtained. We name those: Normal, Reverse, Hybrid and Transpose orthogonality. To characterize these observations, we developed the Orthogonality Index. Going back to the mathematical definition of orthogonality, this factor is the angle formed between the alkane line and the aromatic hydrocarbon line in the chromatographic space. Using this predictive tool, people should be able to choose the best column set and to optimize easily the separation parameters.

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2. Dimandja, J.-M.D. Comprehensive 2-D GC provides high-performance separations in terms of selectivity, sensitivity, speed, and structure. *Anal. Chem.* **76**, 167A–174A (2004).
3. Dimandja, J., Clouden, G. & Colón, I. Standardized test mixture for the characterization of comprehensive two-dimensional gas chromatography columns: the Phillips mix. *J Chromatogr a* **1019**, 261–272 (2003).