Advanced data processing as the unexpected hyphenation to reveal the full potential of GC×GC-TOFMS.

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After 30 years of existence, GC×GC has crossed multiple milestones to become a mature analytical technique. The constant development of modulators and mass spectrometers technology have conducted to a generation of versatile and powerful commercial instruments. Based on these development, GC×GC-MS applications have evolved to become a key player in all kind of untargeted Omics research.

Indeed, GC×GC-MS can now be used to conduct large scale studies, giving full access to its high-resolution power for targeted and mostly untargeted screening. The current challenges are now localized on the data management side, where powerful chemometric tools are required to unlock GC×GC-MS full potential.

In this award presentation, I will discuss our journey towards the development of large scale GC×GC-MS studies and the concomitant development of the data processing solutions. This presentation will summarize the most commonly apply techniques to extract significant information from complex data set. In addition, I will also discuss the key steps of GC×GC-MS data processing workflow and the current tools available. Finally, some future perspectives on the development of the next generation of chemometric tools, especially machine learning, will be discussed.