

## Research Topic for the ParisTech/CSC PhD Program

**Subfield:** Analytical Chemistry applied to medicine and health

**ParisTech School:** ESPCI Paris

**Title:** Identification of disease biomarkers in breath by multidimensional separation techniques

**Advisor(s):** (Jérôme VIAL, Jerome.vial@espci.fr, <https://www.lsabm.espci.fr/spip.php?rubrique8>)

**Short description of possible research topics for a PhD:** (10-15 lines in English + optional figure)

The efficient detection of diseases by trained dogs has been demonstrated recently (KDOG project etc.). In France, 2 dogs have been purchased for this purpose. However, training of dogs is time consuming and expensive. Thus, there is a need for alternative solutions such as the implementation of efficient analytical protocols for this purpose. Such a project requires a full optimization of all the steps before and after the separation itself: before the separation step, the collection of samples must be easy, exhaustive and robust (without discrimination); it must perform some concentration of compounds for trace amount analysis. After the separation, high resolution mass spectrometry must be coupled to the separation technique; this is mandatory for a reliable identification of molecules. In order to be able to perform a detailed analysis (possibly comprehensive) a high resolution separation technique such as UHPLC is mandatory. Multidimensional separation stage cannot be excluded for enhanced separation.

Last but not least, a close collaboration with hospitals (CHU Grenoble, Pitié Salpêtrière, Gustave Roussy are potential partners) will allow the definition of the diseases of interest and the collection of samples. Also, a collaboration with the CEA will provide us with miniaturized devices to be used to perform the preconcentration step of compounds of interest from the breath.

**Required background of the student:** (Which should be the main field of study of the applicant before applying)

An education in separation sciences including liquid chromatography is a prerequisite. A background in mass spectrometry would be perfect.

**A list of 5 (max.) representative publications of the group:** (Related to the research topic)

[1] V. Cuzuel, E. Portas, G. Cognon, I. Rivals, F. Heulard, D. Thiébaud, J. Vial, Sampling method development and optimization in view of human hand odor analysis by thermal desorption coupled with gas chromatography and mass spectrometry, *Anal. Bioanal. Chem.* 409 (2017) 5113–5124. doi:10.1007/s00216-017-0458-8.

[2] L. Sghaier, C.B.Y. Cordella, D.N. Rutledge, M. Watiez, S. Breton, A. Kopczuk, P. Sassiati, D. Thiebaut, J. Vial, Comprehensive Two-dimensional Gas Chromatography for Analysis of the Volatile Compounds and Fishy Odor Off-flavors from Heated Rapeseed Oil, *Chromatographia*. 78 (2015) 805–817. doi:10.1007/s10337-015-2897-8.

[3] R. Al Bakain, I. Rivals, P. Sassiati, D. Thiébaud, M.-C. Hennion, G. Euvrard, J. Vial, Comparison of different statistical approaches to evaluate the orthogonality of chromatographic separations: Application to reverse phase systems, *J. Chromatogr. A*. 1218 (2011) 2963–2975. doi:10.1016/j.chroma.2011.03.031.

[4] V. Cuzuel, A. Sizun, G. Cognon, I. Rivals, F. Heulard, D. Thiébaud, J. Vial, Human odor and forensics. Optimization of a comprehensive two-dimensional gas chromatography method based on orthogonality: How not to choose between criteria, *J. Chromatogr. A*. (2017). doi:10.1016/j.chroma.2017.08.060.

[5] T. H. Chappuis, A. Solgadi, P. Sassiati, J. Vial,† A. Combès, P. Chaminade, D. Thiébaud, Offline two dimensional liquid chromatography with hybrid high resolution mass spectrometry for phospholipid structural determination in lipidomics : Heart cutting vs. comprehensive, in preparation.