



Untargeted metabolomic approach by GC-QTOF : From low to high resolution

Carole Migné, Nils Paulhe, Yann Guitton, Franck Giacomoni, Mélanie Pétéra, Stéphanie Durand, Estelle Pujos-Guillot

► To cite this version:

Carole Migné, Nils Paulhe, Yann Guitton, Franck Giacomoni, Mélanie Pétéra, et al.. Untargeted metabolomic approach by GC-QTOF : From low to high resolution. SMMAP 2017 (Spectrométrie de Masse, Métabolomique et Analyse Protéomique), Oct 2017, Marne-La-Vallée, France. , pp.476, 2017, SMMAP 2017-Livre des résumés. hal-01674479

HAL Id: hal-01674479

<https://hal.science/hal-01674479>

Submitted on 2 Jan 2018

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Untargeted metabolomic approach aims to gather information on as many metabolites as possible in biological systems by taking into account all informations present in the data sets. This approach is essential to pinpoint modifications of metabolic pathways associated to nutritional, health or environmental status for identifying biomarkers.

GC is often coupled to single quadrupole analyzers, which offer high sensitivity, good dynamic range but operate with slower scan rates and lower resolution compared to Time of Flight (ToF) systems. GC coupled with ToF Mass Spectrometry is increasingly used for metabolite profiling because of fast acquisition rates, particularly useful for an accurate deconvolution of overlapping peaks obtained from complex mixtures.



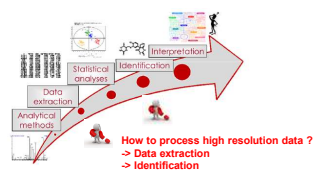
GC-MS 5975 Agilent

	Low Resolution	High Resolution
Sensitivity	-	+
Resolution	-	+
Acquisition Rate	+	++
Databases	NIST, GOLM, FIEHN and in-house databases	MassBank and in-house databases

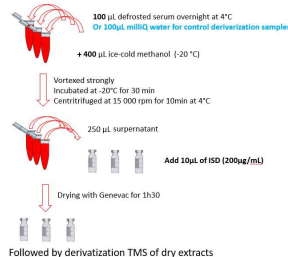


GC-QTOF 7200 Agilent

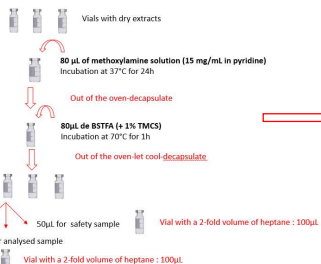
Untargeted metabolomic approach



Sample preparation*



Trimethylsilylation Derivatization*



GC Conditions :

Injection system: 2 µL split 1/20, T = 250 °C.
 Column: HP5-MS (30 m x 0.25 mm x 0.25 µm)
 Carrier gas: He 5.5, 1 mL / min constant debit.

GCMS Analysis*

	Run	Time	MS/MS	MS/MS	MS/MS	MS/MS
Run 1	1	20	100	100	100	100
Run 2	2	20	100	100	100	100
Run 3	3	20	100	100	100	100

Total run time : 49 min

MS Conditions: EI ion source temperature : 230°C, full scan mode (m/z 50-800)

Quad parameters

EI ion source temperature: 230°C
 Quadrupole Temperature: 150°C
 Electron energy: 70eV

ToF parameters

Acquisition 2GHzEDR with N2 (1.5mL/min)
 Acq rate: 5 spectra/s
 Acq time: 200ms/spectrum
 Transients by spectrum: 2712
 Limits for average PPM error: 3.0 and maximum error: 8.0

*Adapted from Gao X. et al, Anal Chem 2010

Bioinformatic tools : Available workflow to process GS-MS data

