

Supplementary material

Identification and quantification of phytoprostanes and phytofurans of coffee and cocoa by- and co-products

Mariana Ruesgas-Ramón^a, Maria Cruz Figueroa-Espinoza^{a,*}, Erwann Durand^{a,b}, Mirna L. Suárez Quiroz^c, Óscar González Ríos^c, Amandine Rocher^d, Guillaume Reversat^d, Joseph Vercauteren^d, Camille Oger^d, Jean-Marie Galano^d, Thierry Durand^d, Claire Vigor^{d,*}.

^a IATE, Univ Montpellier, CIRAD, INRA, Montpellier SupAgro, Montpellier, France.

^b CIRAD, UMR IATE, F-34398 Montpellier, France.

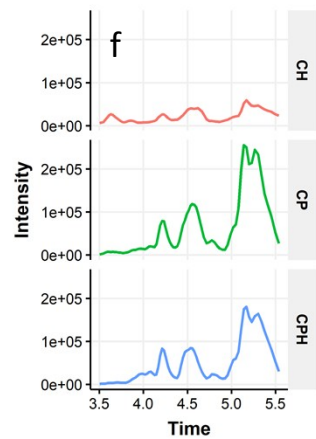
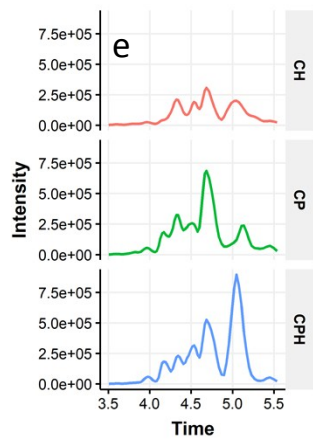
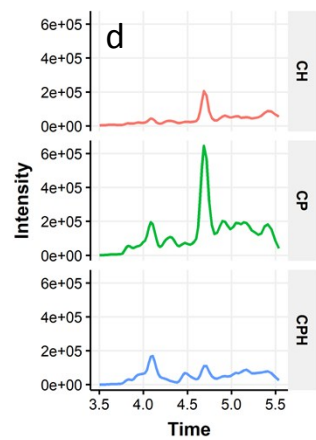
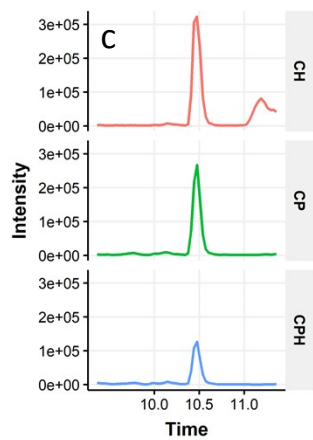
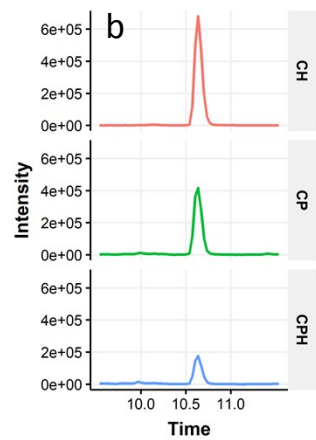
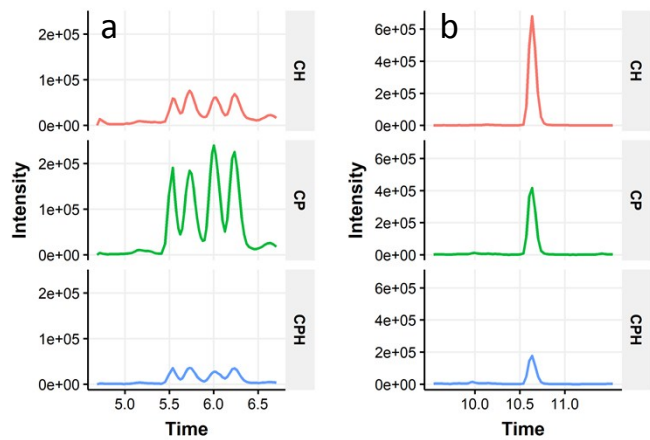
^c Tecnológico Nacional de México/Instituto Tecnológico de Veracruz. UNIDA, Miguel Ángel de Quevedo N° 2779, 91860 Veracruz, Veracruz, México.

^d Institut des Biomolécules Max Mousseron, IBMM, University of Montpellier, CNRS, ENSCM, Faculty of Pharmacy, Montpellier, France.

***Corresponding authors:**

C.V. E-mail: claire.vigor@umontpellier.fr

M.C.F.-E. E-mail: maria.figueroa@supagro.fr



a) *ent*-16-F_{1t}-PhytoP, *ent*-16-*epi*-16-F_{1t}-PhytoP, 9-F_{1t}-PhytoP, 9-*epi*-9-F_{1t}-PhytoP

b) *ent*-9-L_{1t}-PhytoP

c) *ent*-16-B_{1t}-PhytoP

d) *ent*-16(*RS*)-13-*epi*-ST-Δ¹⁴-9-PhytoF

e) *ent*-16(*RS*)-9-*epi*-ST-Δ¹⁴-10-PhytoF

f) *ent*-9(*RS*)-12-*epi*-ST-Δ¹⁰-13-PhytoF

Fig. 1. : Chromatograms acquisition of multiple reaction monitoring (MRM) transitions with “Scheduled MRM mode”

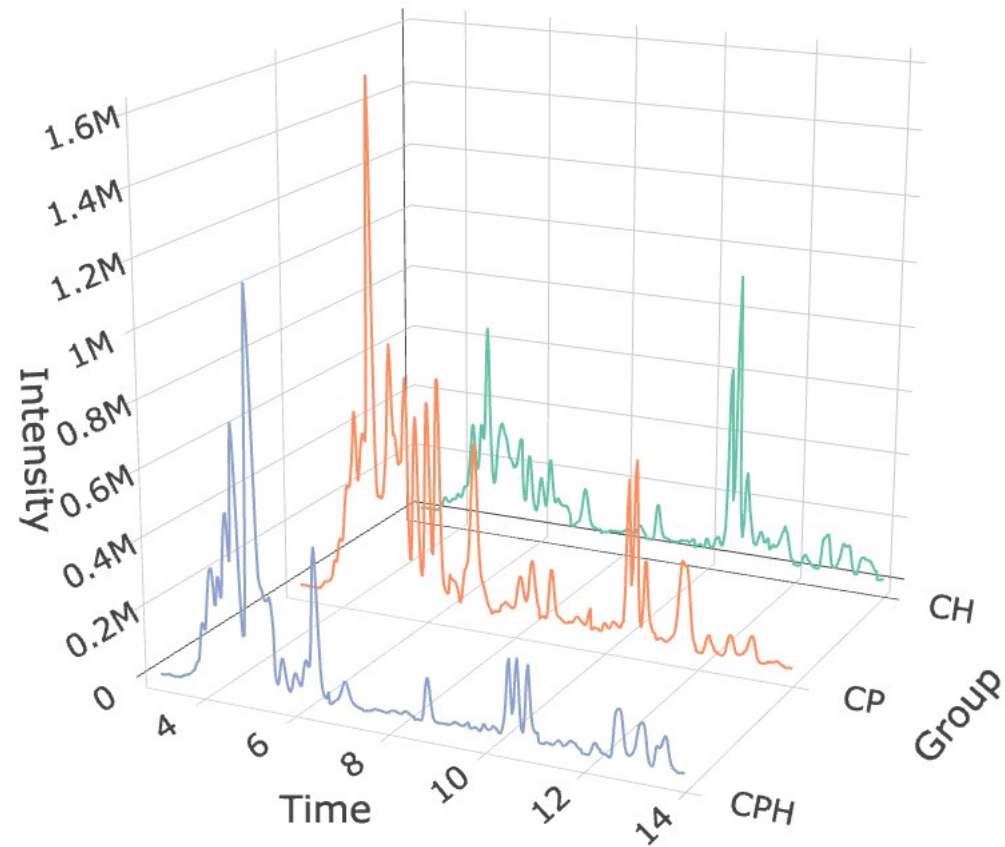


Fig. 2. Total ion current chromatograms of the selected daughter ion mass spectra obtained during micro LC-MS/MS