

# Development of an Online Instrument for Continuous Gaseous PAH Quantification: Laboratory Evaluation and Comparison with The Offline Reference UHPLC-Fluorescence Method

Joana Vaz-Ramos <sup>1,2</sup>, Mathilde Mascles <sup>3</sup>, Anaïs Becker <sup>1</sup>, Damien Bourgain <sup>3</sup>, Audrey Grandjean <sup>1,3</sup>, Sylvie Bégin-Colin <sup>2</sup>, Franck Amiet <sup>3</sup>, Damien Bazin <sup>3</sup>, and Stéphane Le Calvé <sup>1,\*</sup>

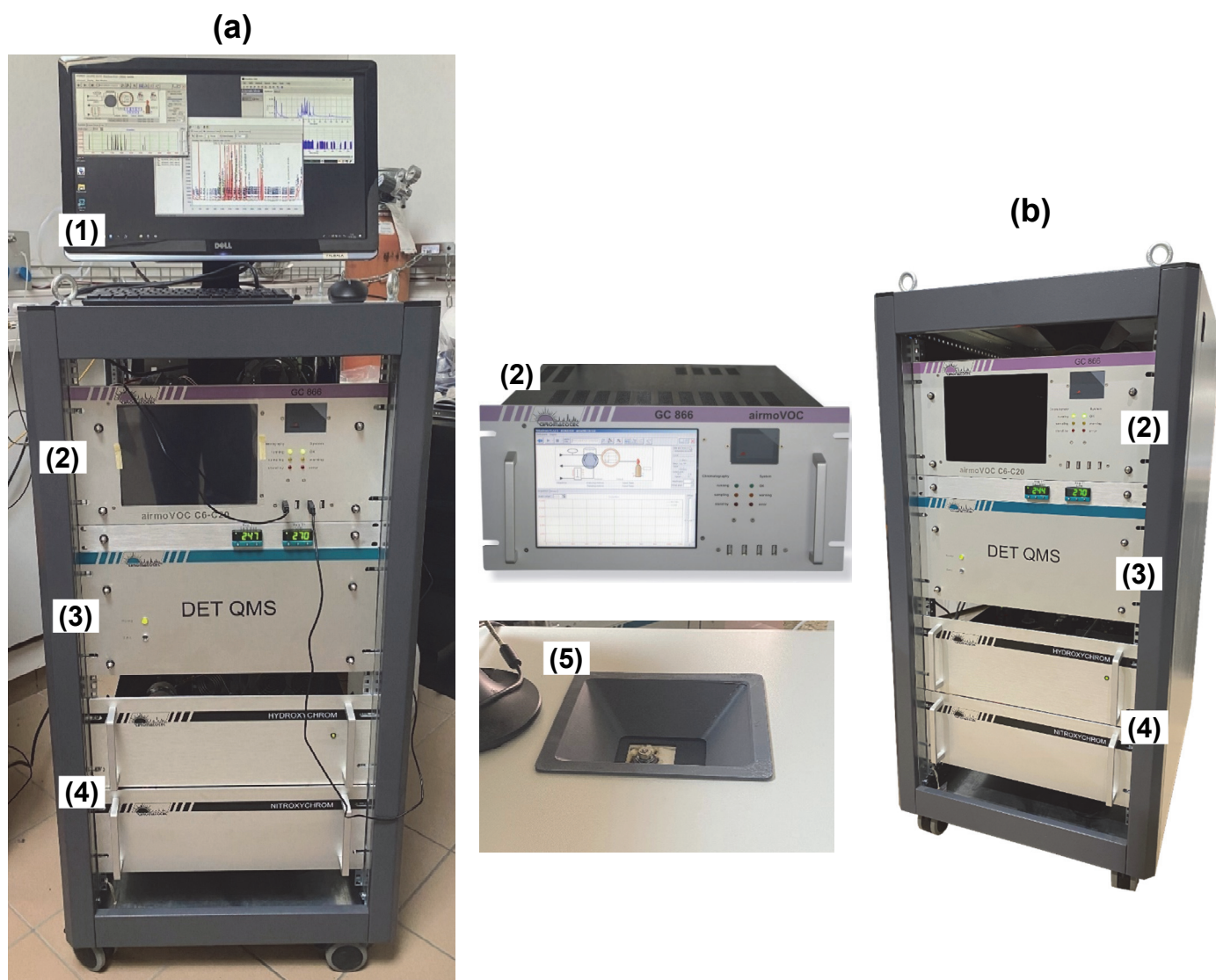
<sup>1</sup> Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé (ICPEES), UMR-7515 CNRS-Université de Strasbourg, 25 Rue Becquerel, 67087 Strasbourg, France; joana.vazramos@ipcms.unistra.fr (J.V.-R.); ana.becker@unistra.fr (A.B.); audrey.grandjean@chromatotec.com (A.G.)

<sup>2</sup> Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), UMR-7504 CNRS-Université de Strasbourg, 23 Rue du Loess, 67034 Strasbourg, France; sylvie.begin@unistra.fr

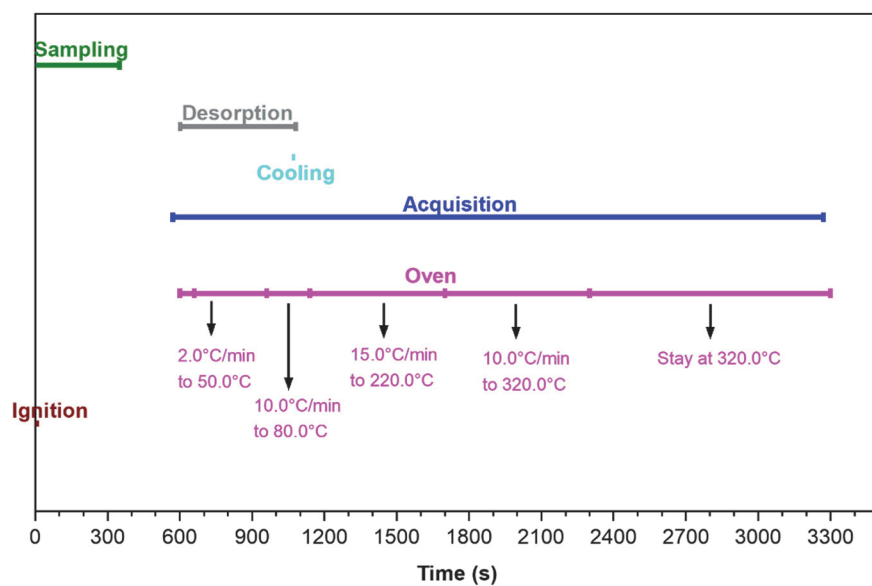
<sup>3</sup> Chromatotec, 15 Rue d'Artiguelongue, 33240 Saint-Antoine, France; mathilde.mascles@chromatotec.com (M.M.); damien.bourgain@chromatotec.com (D.B.); franck.amiet@chromatotec.com (F.A.); damien.bazin@chromatotec.com (D.B.)

\* Correspondence: slecalve@unistra.fr

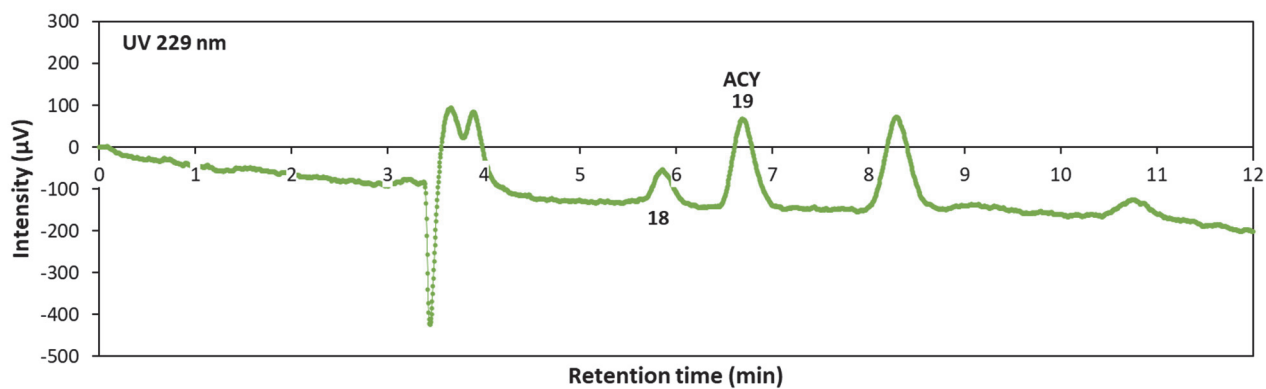
## Supplementary Information



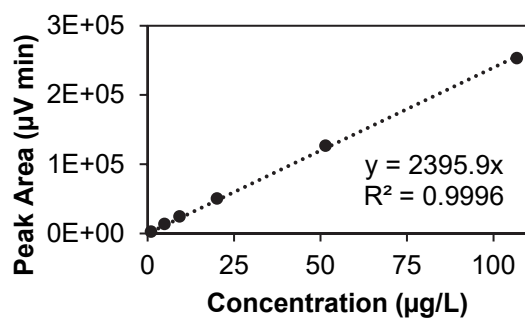
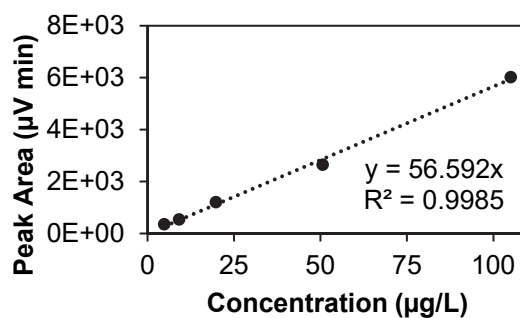
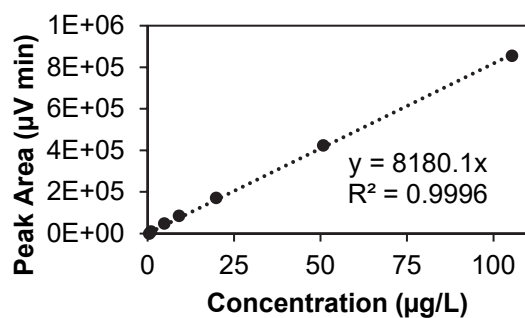
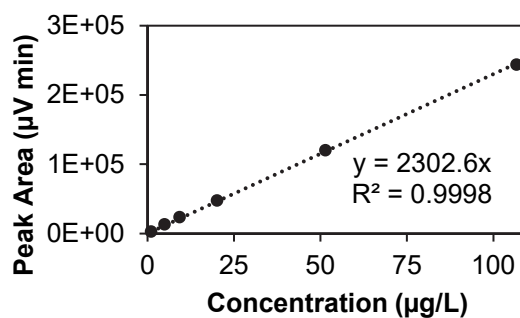
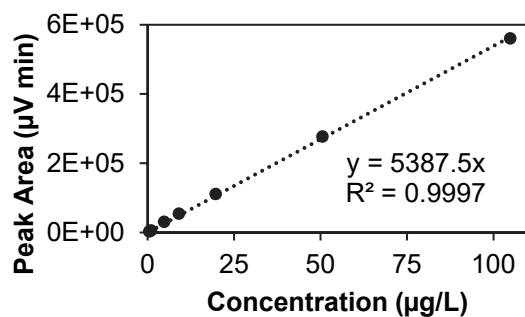
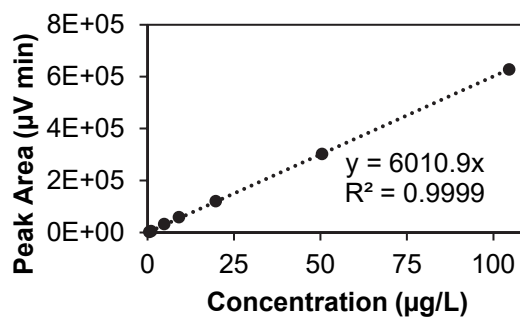
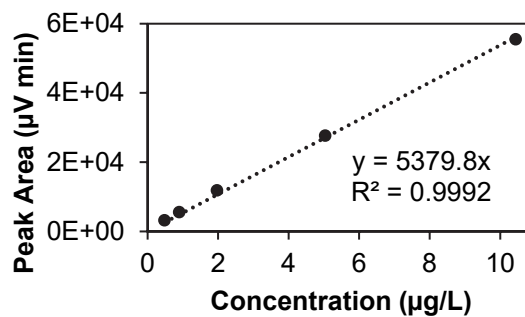
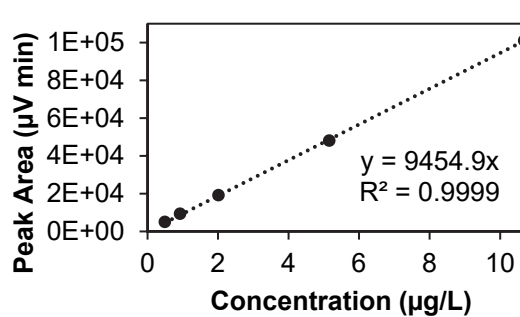
**Figure S1.** Photo of the instrument airmo C6-C20+ used for the GC-FID method: (a) general view of the instrument in-place and operational, and (b) sideview. Different units of the instrument are highlighted: (1) computer interface; (2) airmo C6-C20+ unit; (3) mass spectrometer (not used in this application); (4) hydroxychrom - hydrogen generator; and (5) injector.

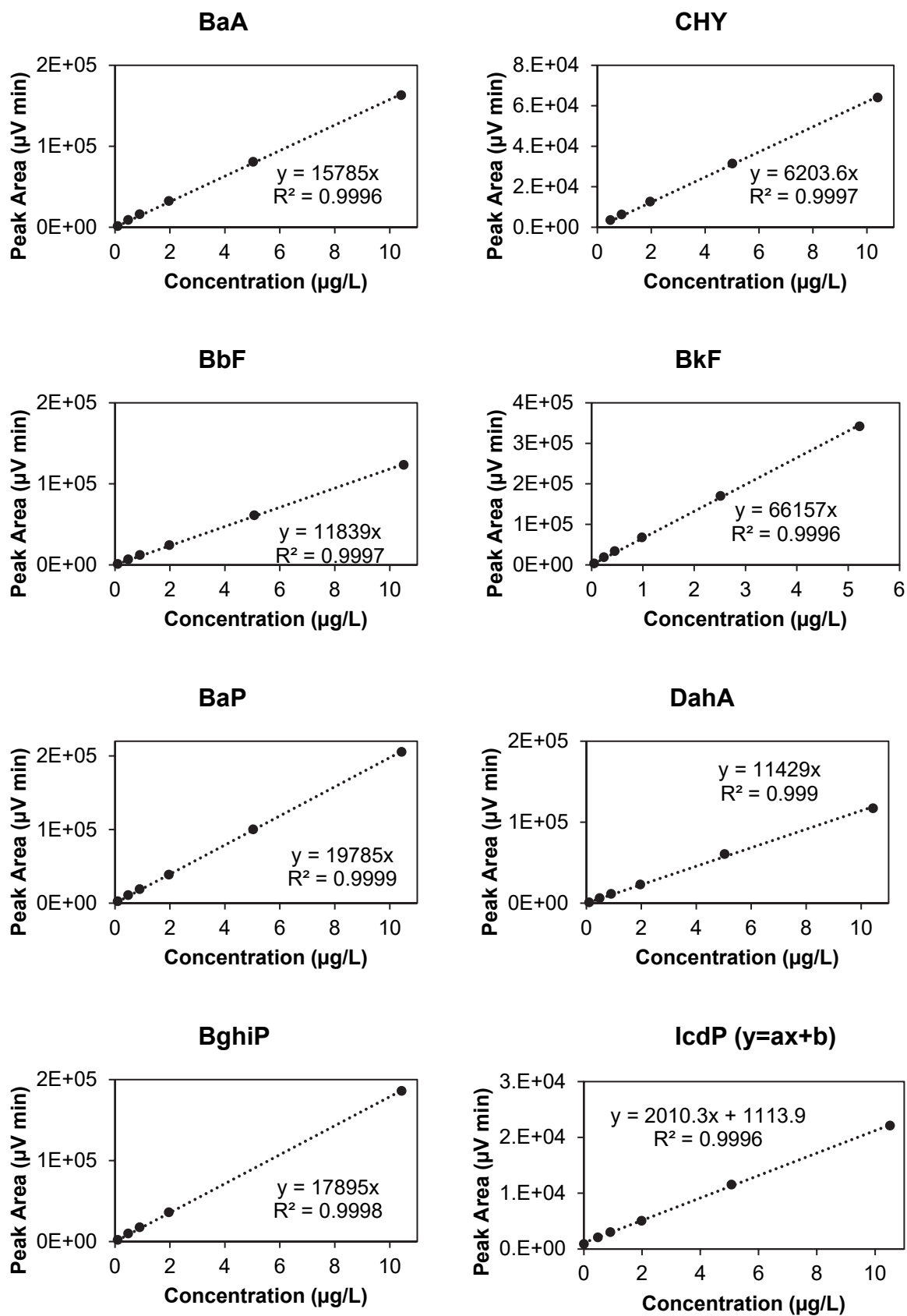


**Figure S2.** Time events of the GC-FID method.

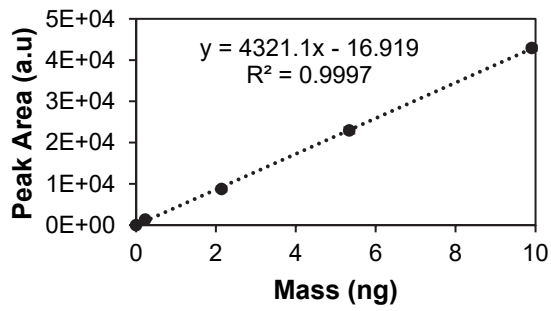
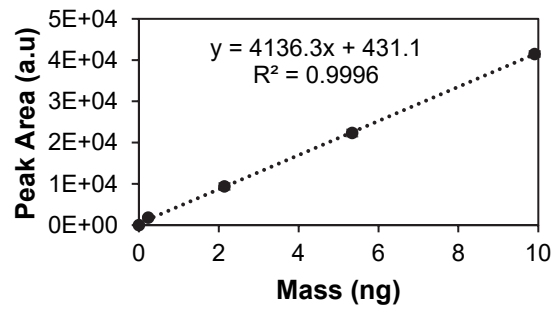
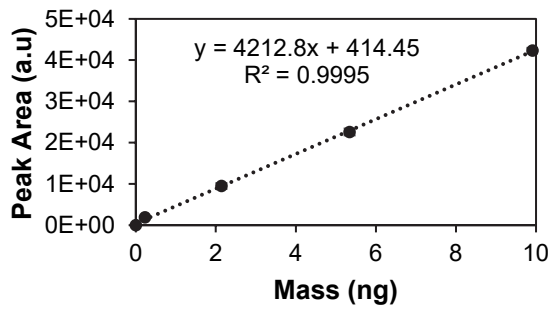
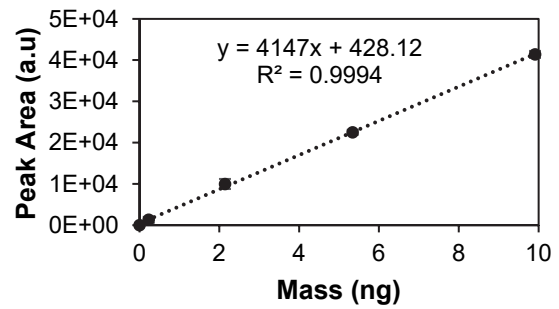
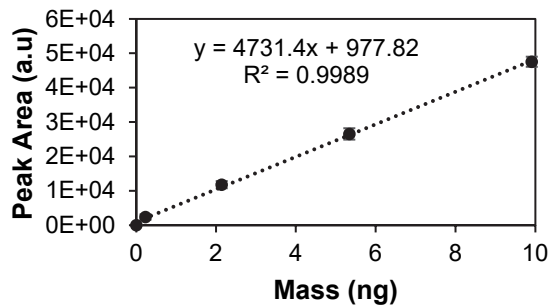
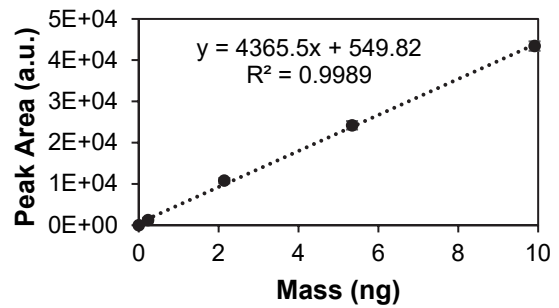
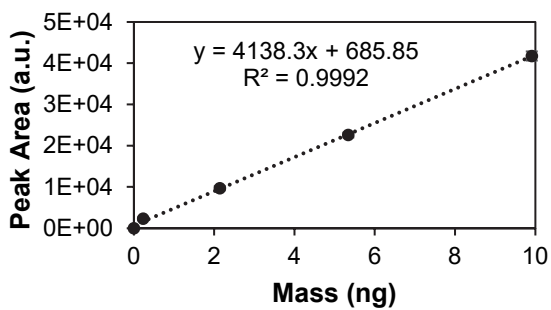
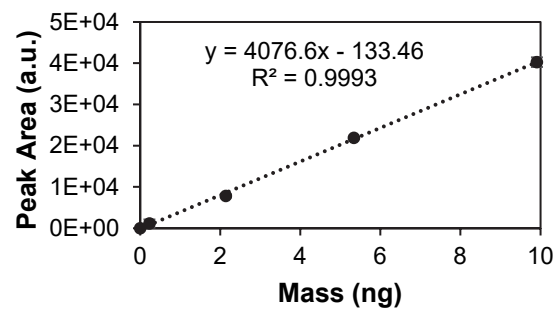


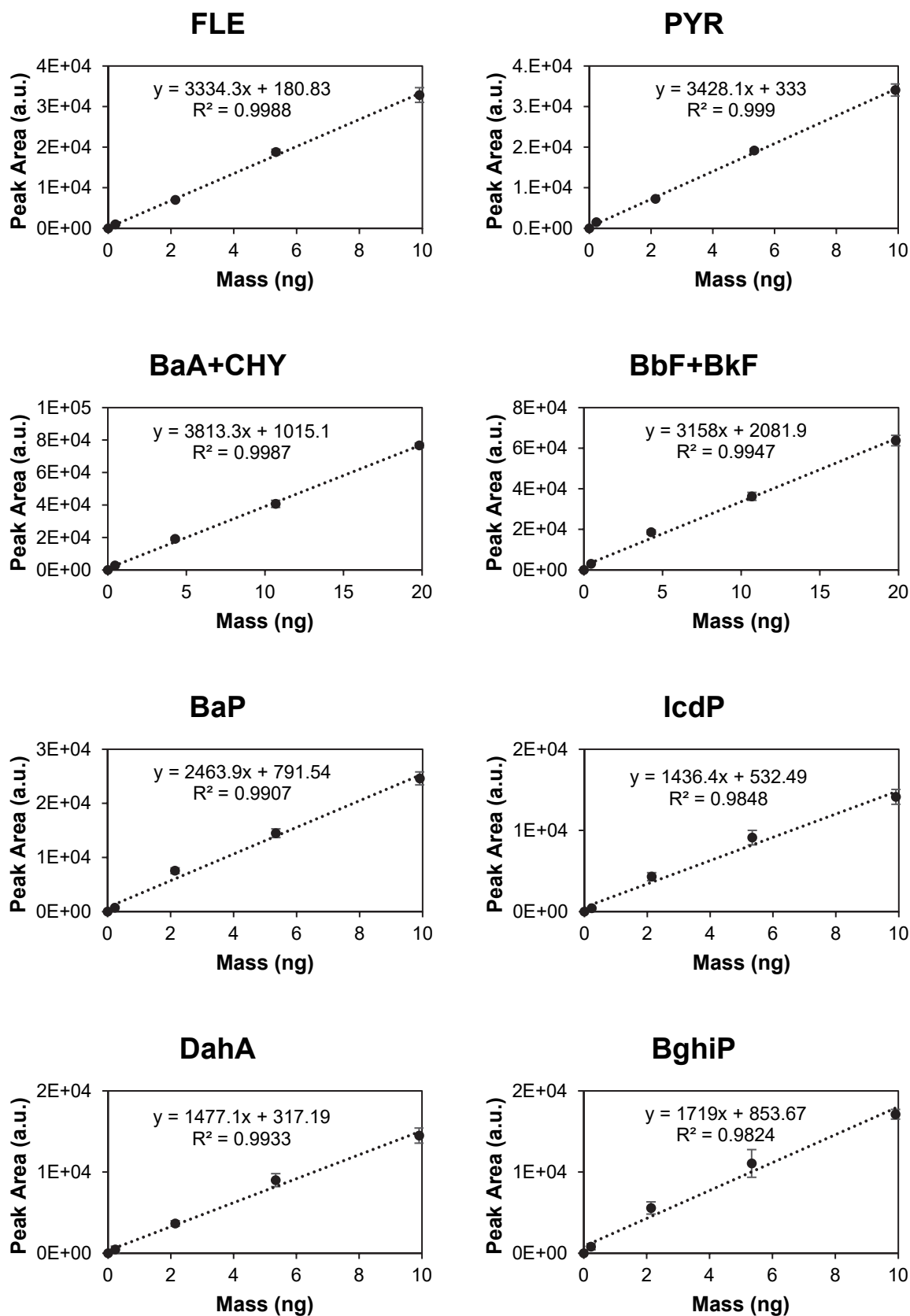
**Figure S3.** Chromatogram the developed UHPLC-FLD/UV method for the UV detection at 229 nm, obtained with an injection volume of 2  $\mu$ L and a PAH concentration of 2.52 (BkF) to 51.48 (NAP)  $\mu$ g/L depending on the PAH. Peak 19 corresponds to acenaphthylene (ACY), while peak 18 is naphtalene (NAP).

**NAP****ACY****ACE****FLU****PHE****ANT****FLE****PYR**



**Figure S4.** Calibration curves for the 16 US EPA PAH were obtained with the UHPLC-FLD/UV method, using a gradient of ACN : Water from 45 : 55 up to 0 : 100 as mobile phase, an oven temperature of 30°C and an injection volume of 2 μL. The dashed line corresponds to the linear regression in the investigated concentration ranges 0.5 – 100 μg/L, 0.5 – 10 μg/L and 0.5 – 5 μg/L, depending on the PAH.

**NAP****2-Me-NAP****1Me-NAP****ACE****ACY****FLU****PHE****ANT**



**Figure S5.** Chromatographic peak area versus PAH mass injected at the GC injector of airmoVOC C6–C20+ instrument (GC-FID method), allowing vaporization of PAH to mimic gas phase concentrations. The dashed line corresponds to the linear regression in the investigated concentration range, i.e., between 0 and 9.91 ng for all the PAH. These PAH masses were obtained by injecting 1 µg/L of a standard PAHs mixture solution of 0 – 9.9 µg/mL. Because



of their co-elutions, the pairs BkF + BbF and BaA + CHY were quantified together. The vertical error bars correspond to the standard deviation of the peak area determined from triplicates.