SUPPLEMENTARY MATERIALS

Experimental Design and Multiple Response Optimization for the Extraction and Quantitation of Thirty-four Priority Organic Micropollutants in Tomatoes through the QuEChERS Approach

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Figure S1. Visual results of the extraction of "Rio Grande" cultivar using cyclohexane (A), acetone (B) and dichloromethane (C) solvents. 0.5 g sample weight, 10 mL extraction volume and 5 min @ 1507xg centrifuge.
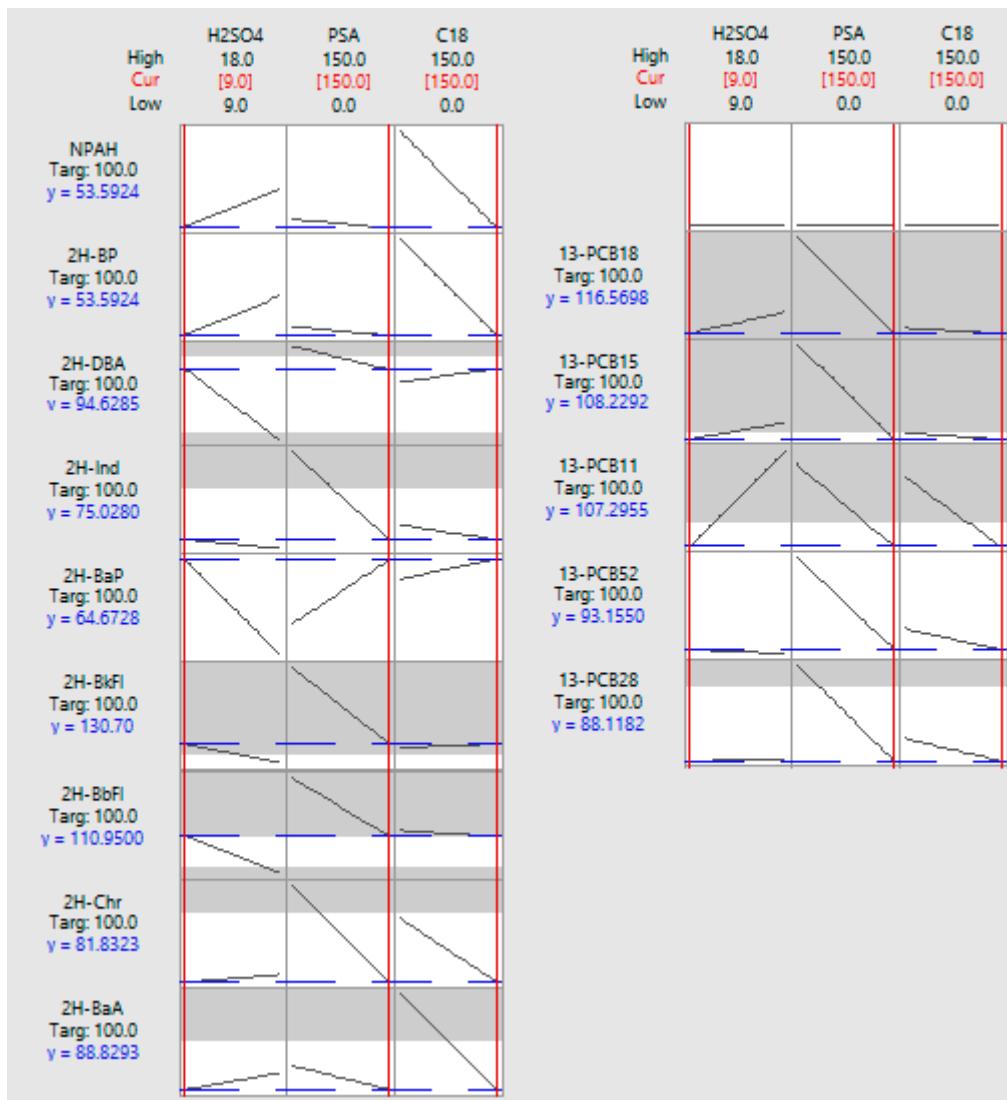

Figure S2. The optimization plot retrieved from MiniTab software, after performing the multiple response optimization. The optimization plot shows the effect of each factor (columns) on the responses or composite desirability (rows). The vertical red lines on the graph represent the current factor settings. The numbers

displayed at the top of a column show the current factor level settings (in red). The horizontal blue lines and numbers represent the responses for the current factor level.
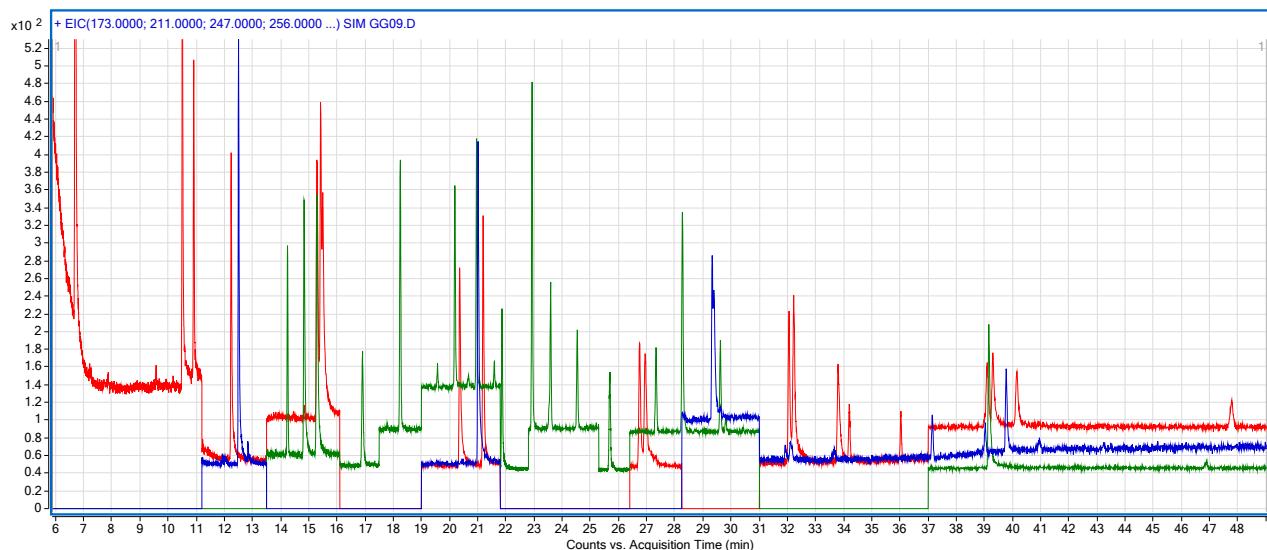

Figure S3. Total ion chromatogram obtained for the 16 PAHs (red line), 14PCBs (green line) and 4 nitro-PAHs (blue line) in post-extraction solvent using the optimized QuEChERS approach followed by GC-MS. Analysis conditions are detailed in Material and Method section.
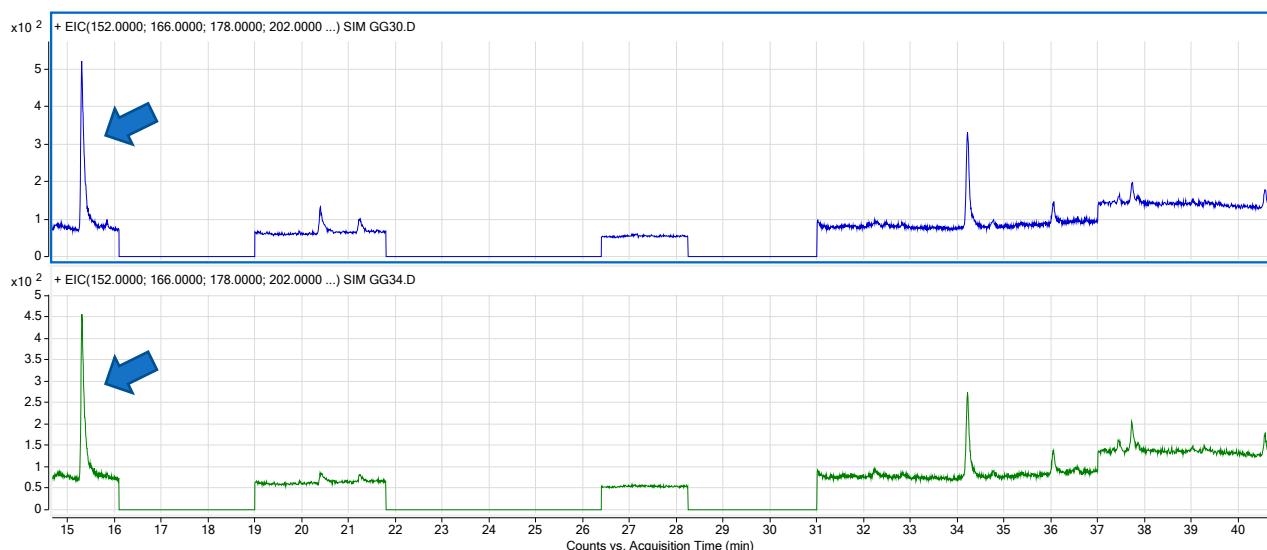

Figure S4. Chromatograms obtained after the extraction and analysis of "Rio Grande" (blue) and "Beefsteak" (green) using the optimized protocol. Phe peak is evidenced by a blue arrow. Protocols details are reported in Material and Method section.

Table S1. Equation models and histogram of coefficients retrieved for each surrogate after the full factorial design (conditions detailed in paragraph 3.1.2.1)

Analyte	Equation and diagram

BaA-d$_{12}$

$$BaA\text{-}d_{12}=256,9-7,30\times H_2SO_4-0,745\times PSA-$$
$$0,752\times C18+0,0385\times H_2SO_4\times PSA+0,0155\times H_2SO_4\times C18+0,00218\times PSA\times C18$$

BaA-d$_{12}$
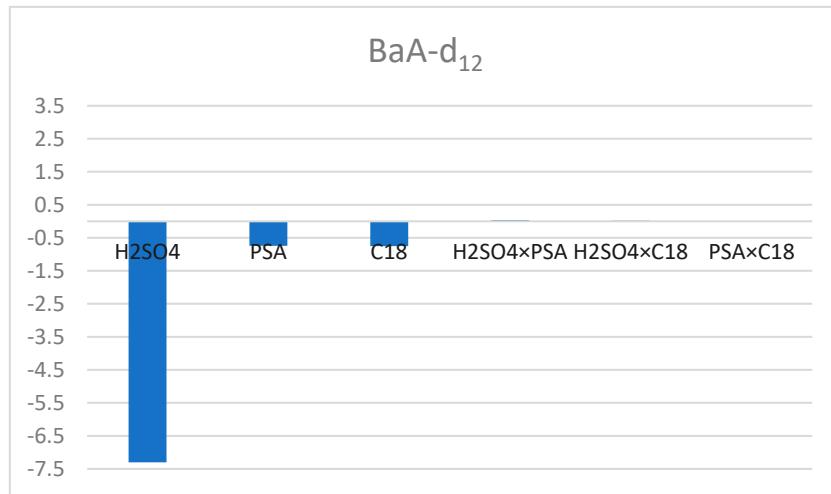
Chr-d$_{12}$

$$Chr\text{-}d_{12}\text{-}=196,1-1,90\times H_2SO_4-0,642\times PSA-0,339\times C18+0,0191\times H_2SO_4\times PSA-$$
$$0,0041\times H_2SO_4\times C18+0,001321\times PSA\times C18$$

Chr-d$_{12}$
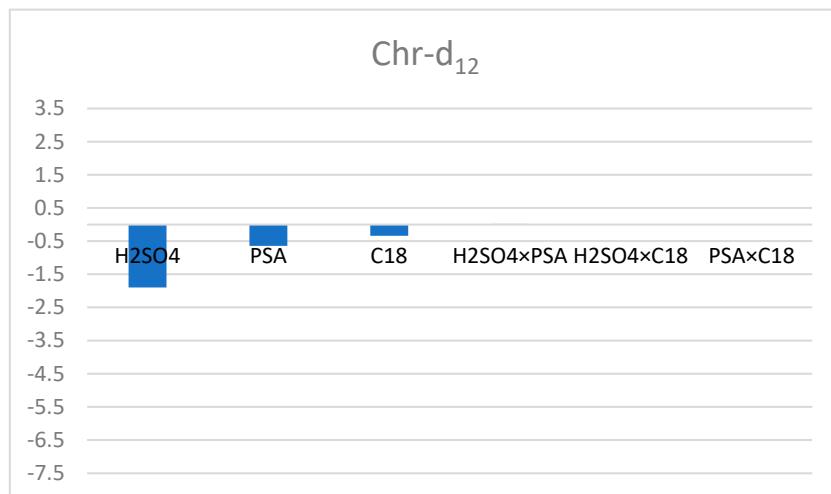
BbFl-d$_{12}$

$$BbF\text{-}d_{12}=247,0-0,30\times H_2SO_4-1,005\times PSA\text{-}+0,004\times C18+0,0180\times H_2SO_4\times PSA-$$
$$0,0489\times H_2SO_4\times C18+0,00260\times PSA\times C18$$

BbFl-d$_{12}$
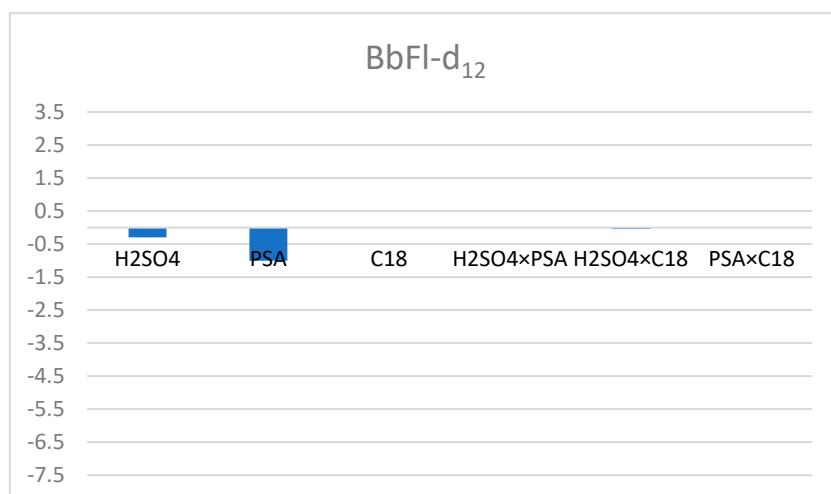
BkFl-d$_{12}$ BkFl-d$_{12}$=250+0,09×H$_2$SO$_4$-1,08×PSA+0,52×C18+0,0270×H$_2$SO$_4$×PSA-

0,0512×H$_2$SO$_4$×C18-0,00012×PSA×C18
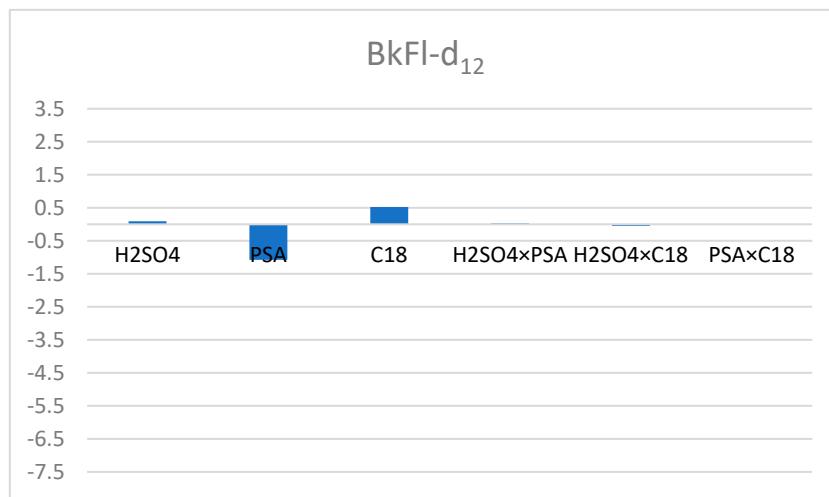
BaP-d$_{12}$ BaP-d$_{12}$=15,42+1,105×H$_2$SO$_4$+0,3538×PSA+0,2258×C18-0,02304×H$_2$SO$_4$×PSA-

0,02527×H$_2$SO$_4$×C18+0,000435×PSA×C18
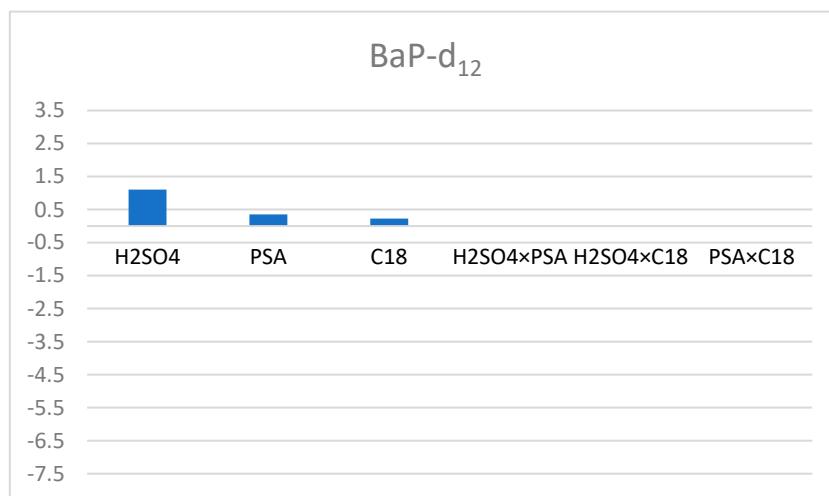
Ind-d$_{12}$ Ind-d$_{12}$=172,7+1,17×H$_2$SO$_4$-0,952×PSA+0,080×C18+0,0328×H$_2$SO$_4$×PSA-

0,0452×H$_2$SO$_4$×C18+0,001745×PSA×C18
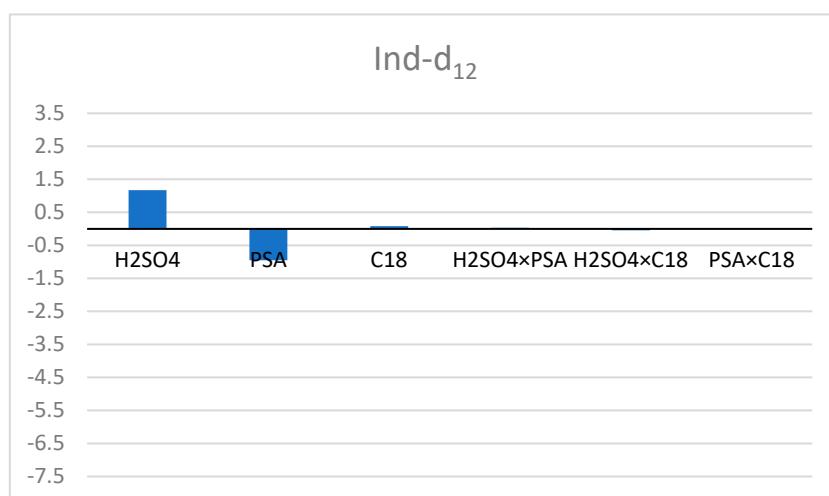
DBA-d$_{14}$ DBA-d$_{14}$=181,6+3,25×H_2SO_4-0,925×PSA+0,252×C18+0,0021×H_2SO_4×PSA-

0,0934×H_2SO_4×C18+0,00469×PSA×C18
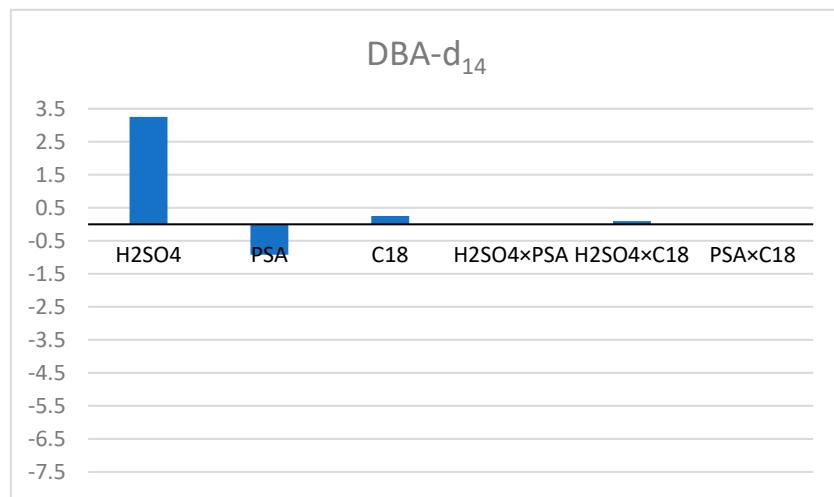
BP-d$_{12}$ BP-d$_{12}$=97,7+4,24×H_2SO_4-0,095×PSA-

0,304×C18+0,0048×H_2SO_4×PSA+0,0111×H_2SO_4×C18+0,00024×PSA×C18
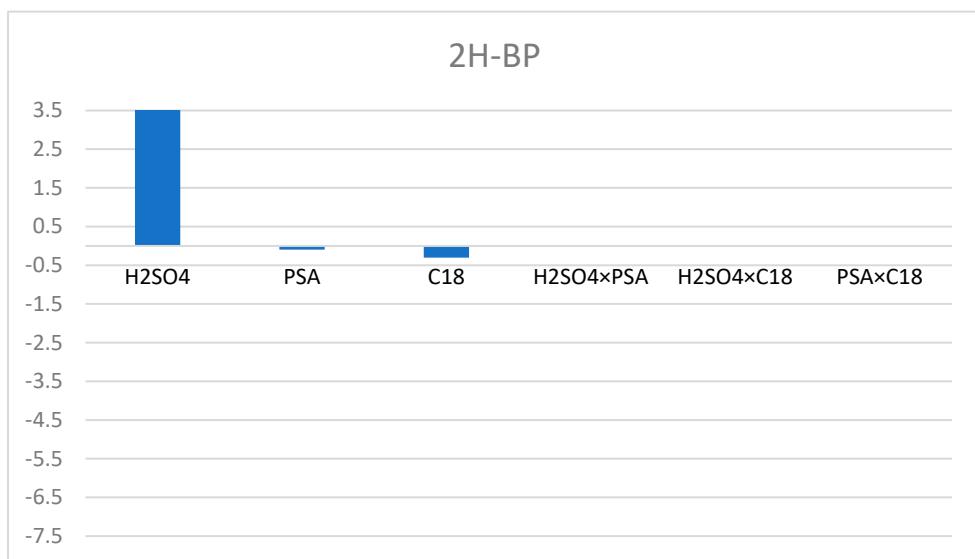
1-Nitropyrene-d$_9$

$$\text{1-Nitropyrene-d}_9 = 97{,}7 - 1{,}24 \times \text{H}_2\text{SO}_4 - 0{,}095 \times \text{PSA} - 0{,}304 \times \text{C18} + 0{,}0048 \times \text{H}_2\text{SO}_4 \times \text{PSA} + 0{,}0111 \times \text{H}_2\text{SO}_4 \times \text{C18} + 0{,}00024 \times \text{PSA} \times \text{C18}$$
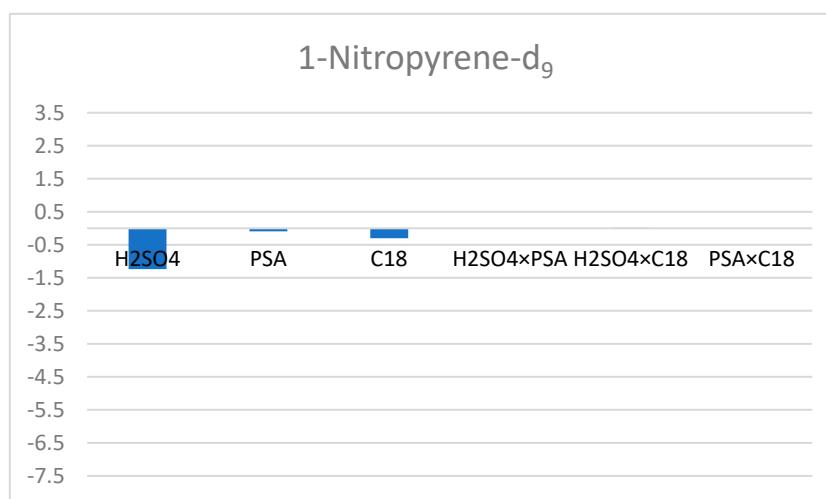

$^{13}\text{C}_{12}$-PCB28

$$^{13}\text{C}_{12}\text{-PCB28} = 126{,}0 - 1{,}07 \times \text{H}_2\text{SO}_4 - 0{,}262 \times \text{PSA} + 0{,}051 \times \text{C18} + 0{,}01321 \times \text{H}_2\text{SO}_4 \times \text{PSA} - 0{,}00550 \times \text{H}_2\text{SO}_4 \times \text{C18} - 0{,}000312 \times \text{PSA} \times \text{C18}$$
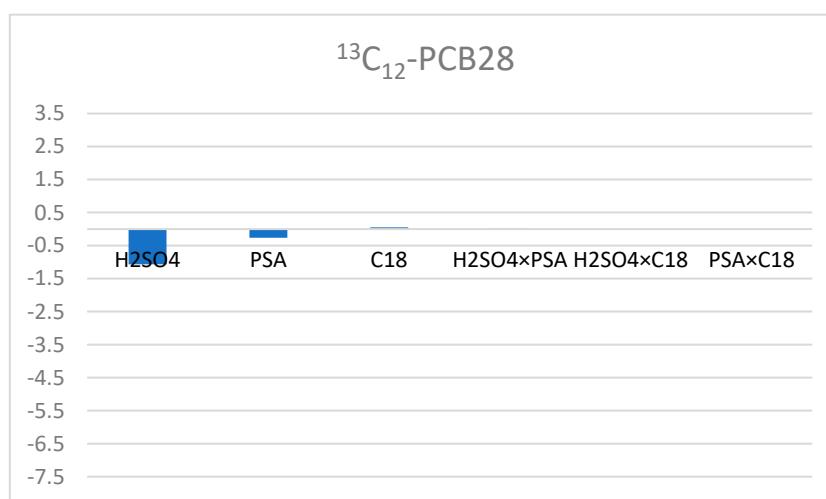

$^{13}\text{C}_{12}$-PCB52

$$^{13}\text{C}_{12}\text{-PCB52} = 116{,}2 + 0{,}07 \times \text{H}_2\text{SO}_4 - 0{,}187 \times \text{PSA} + 0{,}018 \times \text{C18} + 0{,}00608 \times \text{H}_2\text{SO}_4 \times \text{PSA} - 0{,}00712 \times \text{H}_2\text{SO}_4 \times \text{C18} + 0{,}000137 \times \text{PSA} \times \text{C18}$$
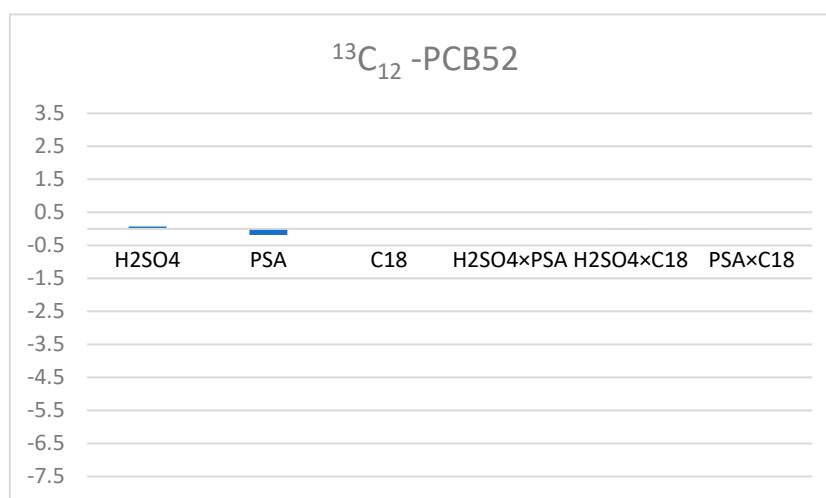
$^{13}C_{12}$-PCB118

$$^{13}C_{12}\text{-PCB118}=134,9-0,585\times H_2SO_4-0,1209\times PSA-0,1592\times C18+0,00427\times H_2SO_4\times PSA+0,00982\times H_2SO_4\times C18+0,000030\times PSA\times C18$$
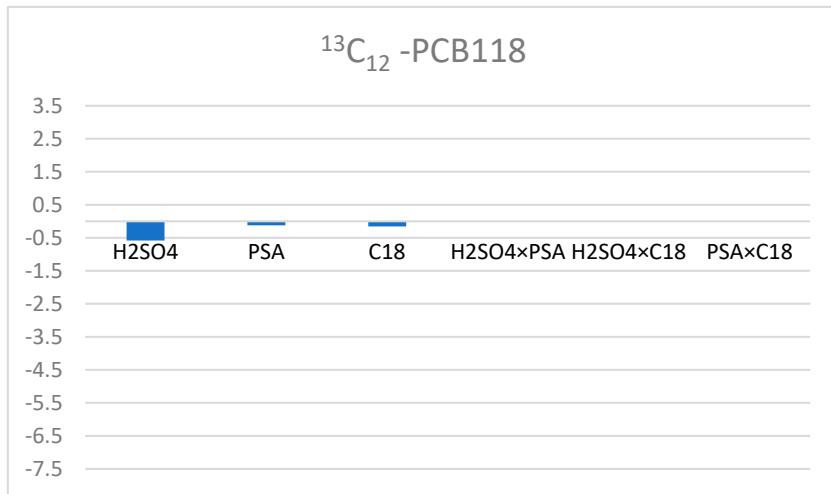
$^{13}C_{12}$-PCB153

$$^{13}C_{12}\text{-PCB153}=133,38-0,299\times H_2SO_4-0,2655\times PSA+0,1009\times C18+0,01404\times H_2SO_4\times PSA-0,00865\times H_2SO_4\times C18-0,000224\times PSA\times C18$$
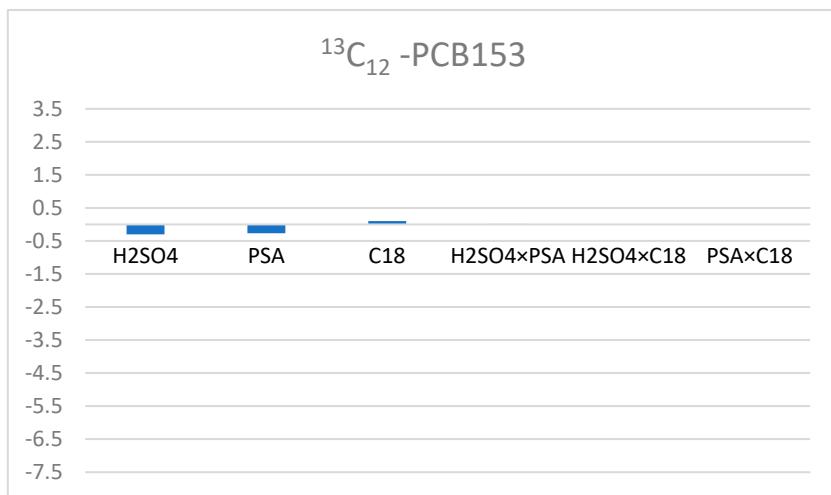
$^{13}C_{12}$-PCB180 $^{13}C_{12}$-PCB180=122,2+3,10×H_2SO_4-0,236×PSA+0,133×C18+0,0026×H_2SO_4×PSA-

0,0186×H_2SO_4×C18+0,00016×PSA×C18
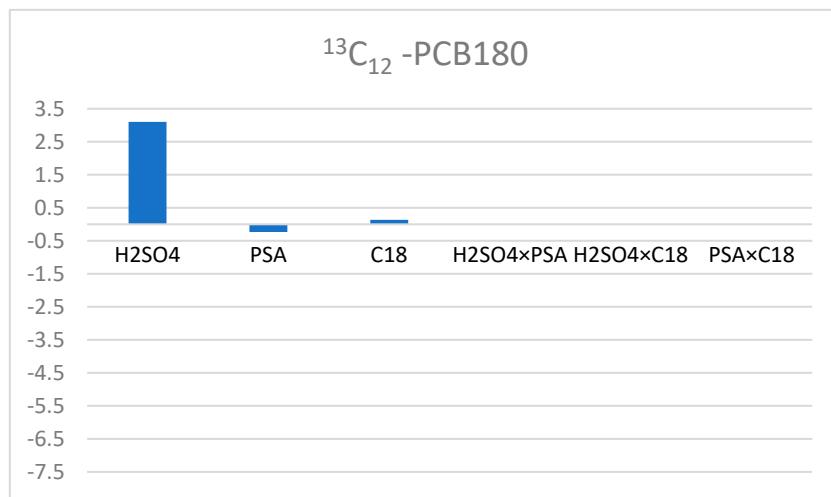
Table S2. Extraction recovery percentages of surrogates from "*Rio Grande*", "*Beefsteak*" and "*Vine*" cultivars. Extraction conditions are detailed in paragraph 2.4.4 of the manuscript.

	Rio Grande	Beefsteak	Vine
BaA -d_{12}	100	102	93
Chr -d_{12}	86	102	81
BbFl -d_{12}	102	91	89
BkFl -d_{12}	108	110	102
BaP -d_{12}	75	62	61
Ind -d_{12}	80	76	86
DBA -d_{14}	81	88	97
BP -d_{12}	60	62	62
1-nitropyrene-d_9	60	74	83
$^{13}C_{12}$-PCB28	86	91	91
$^{13}C_{12}$-PCB52	91	95	98
$^{13}C_{12}$-PCB118	105	104	109
$^{13}C_{12}$-PCB153	107	110	108
$^{13}C_{12}$-PCB180	110	111	110