A new and efficient Solid Phase Microextraction approach for analysis of high fat content food samples using a matrix-compatible coating

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Supporting Information

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Figure captions

Figure S1. Glass liner of the 1079 Split/Splitless Injector contaminated by greasy, non-volatile compounds from avocado puree samples.

Figure S2. Effect of pre-desorption rinsing solvent on analytes stability in the SPME coating

Figure S3: Response variability calculated as RSD% for PDMS/DVB (n=50) and PDMS/DVB/PDMS (n=100).

Figure S4: Response of QC analysis for PDMS/DVB/PDMS and PDMS/DVB used respectively for n=100 and n=50 extractions from avocado puree, before and after manual cleaning.

Figure S1

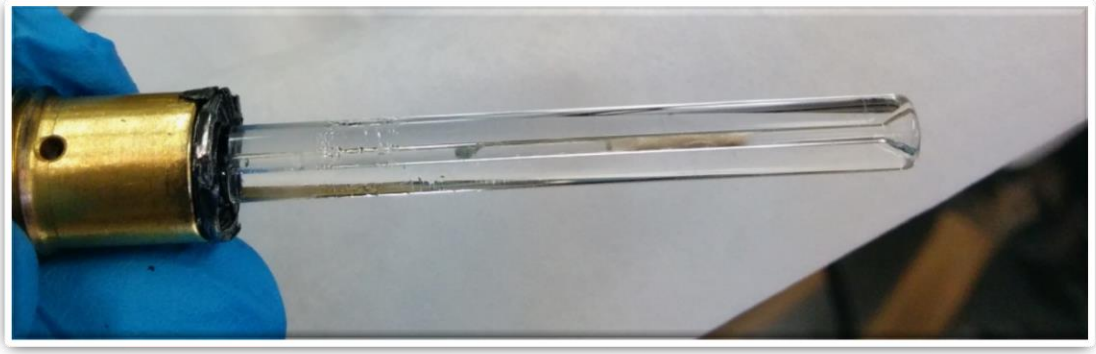


Figure S2

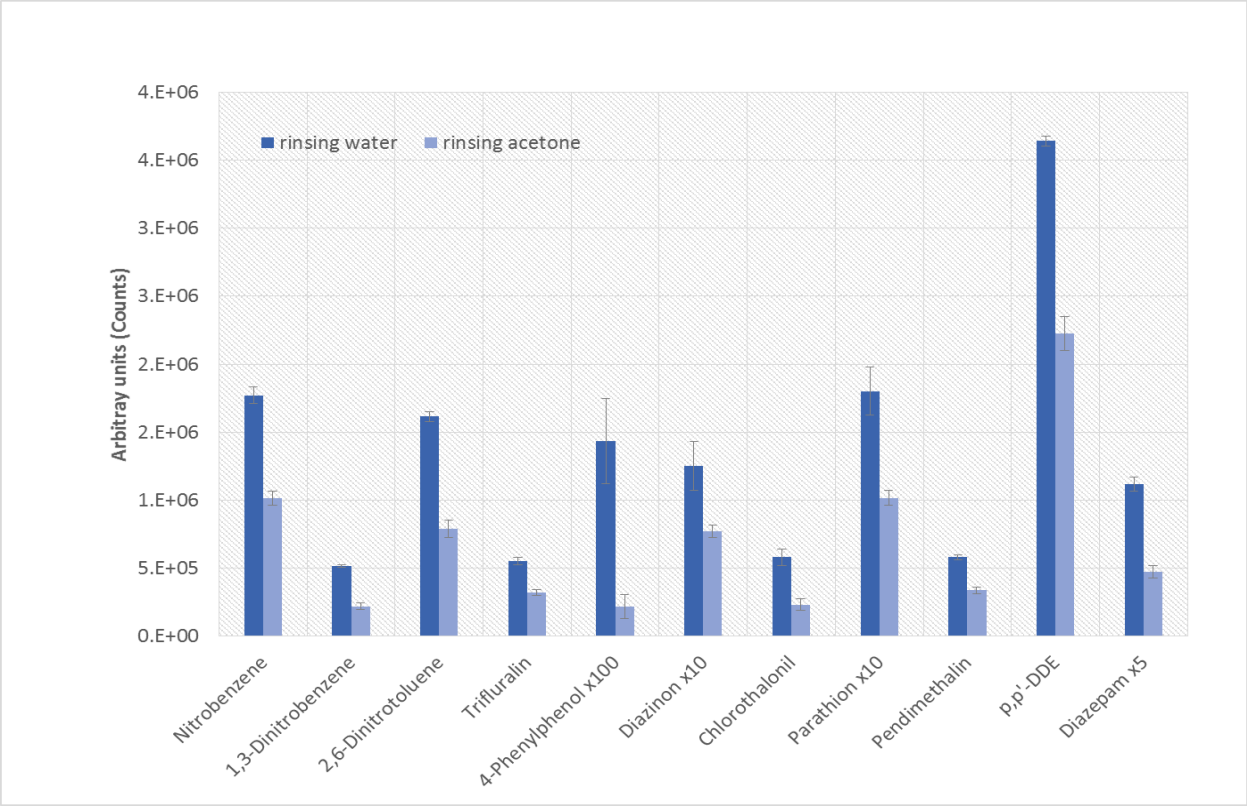

4.E+06
4.E+06
3.E+06
3.E+06
2.E+06
2.E+06
1.E+06
5.E+05
0.E+00
Arbitray units (Counts)
rinsing water
rinsing acetone
Nitrobenzene
1,3-Dinitrobenzene
2,6-Dinitrotoluene
Trifluralin
4-Phenylphenol x100
Diazinon x10
Chlorothalonil
Parathion x10
Pendimethalin
p,p'-DDE
Diazepam x5

Figure S3

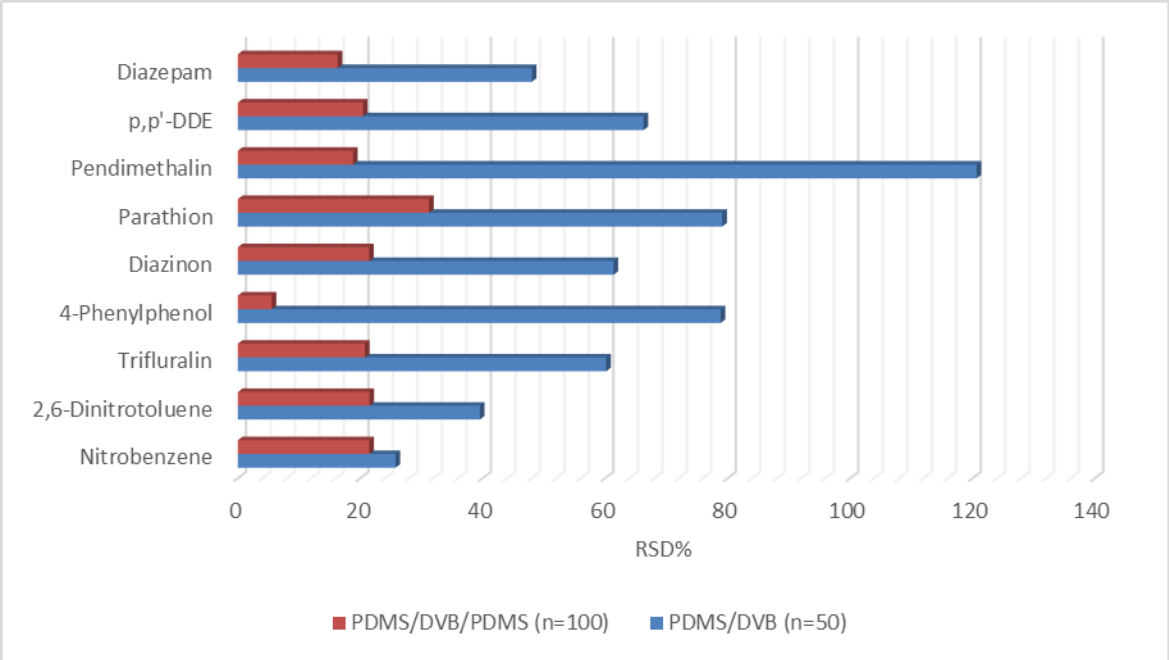

Diazepam
p,p'-DDE
Pendimethalin
Parathion
Diazinon
4-Phenylphenol
Trifluralin
2,6-Dinitrotoluene
Nitrobenzene
0
20
40
60
80
100
120
140
RSD%
PDMS/DVB/PDMS (n=100)
PDMS/DVB (n=50)

Figure S4

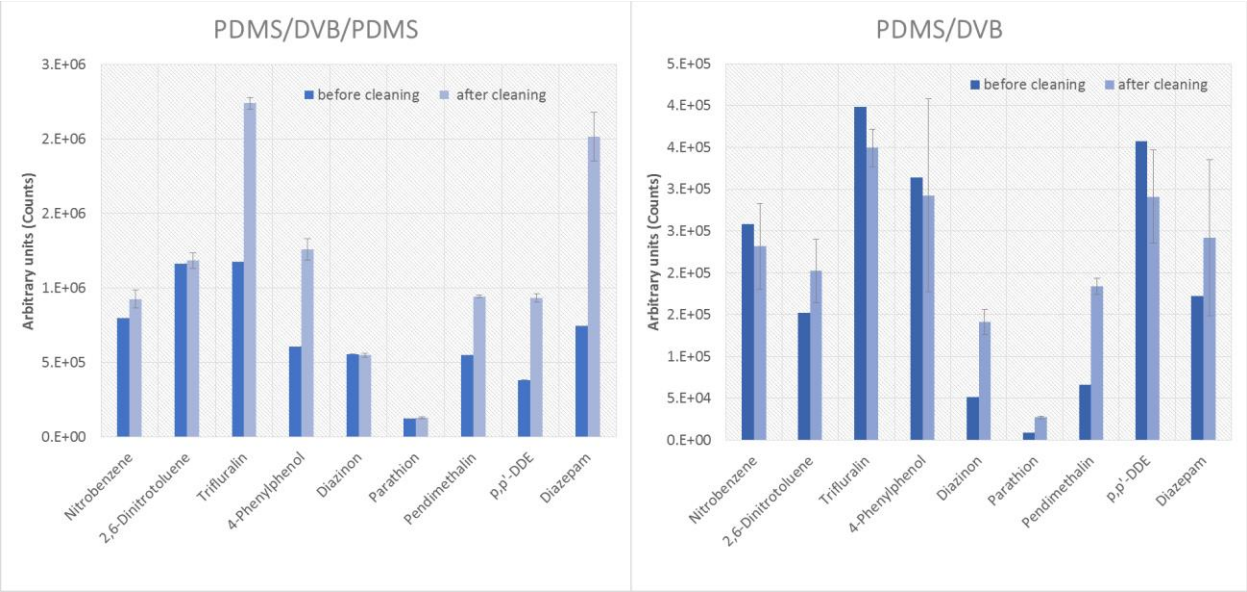

PDMS/DVB/PDMS
Arbitrary units (Counts)
3.E+06
2.E+06
2.E+06
1.E+06
5.E+05
0.E+00
before cleaning
after cleaning
Nitrobenzene
2,6-Dinitrotoluene
Trifluralin
4-Phenylphenol
Diazinon
Parathion
Pendimethalin
p,p'-DDE
Diazepam
PDMS/DVB
Arbitrary units (Counts)
5.E+05
4.E+05
4.E+05
3.E+05
3.E+05
2.E+05
1.E+05
5.E+04
0.E+00
before cleaning
after cleaning
Nitrobenzene
2,6-Dinitrotoluene
Trifluralin
4-Phenylphenol
Diazinon
Parathion
Pendimethalin
p,p'-DDE
Diazepam

Table S1. Target analytes and their physicochemical properties: molecular weight, log P, Henry`s law constant.

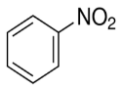
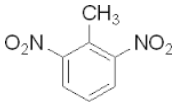
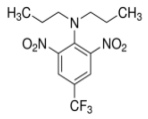
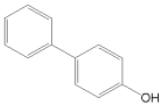
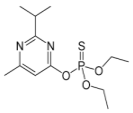
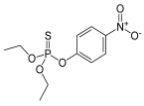
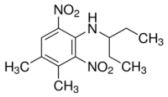
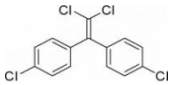
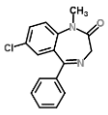
Compound	***Log P (pH 7)***	***Boiling point (°C)***	***Henry's Law constant (atm x m³/mol)***	***Chemical structure***
Nitrobenzene	1.90	210.9	$2.40x10^{-05}$	
2,6-dinitrotoluene	2.42	285	$7.47x10^{-07}$	
Trifluralin	5.07	139.5	$3,9\ x10^{-5}$	
4-phenylphenol	3.20	305-308	$5.23x10^{-8}$	
Diazinon	3.40	306	$1,13x10^{-7}$	
Parathion	3.83	375	$1,0x10^{-7}$	
Pendimethalin	5.18	330	$2,69x10^{-5}$	
p,p'-DDE	6.00	336	$2.1x10^{-5}$	
Diazepam	2.91	497	$3.6x10^{-9}$	

Table S2: Linear retention index of volatiles determined in avocado by means of SPME-GC-MS

Compound	*LRI exp*	*LRI Lit*
3-Methyl butanal	716	702
Hexanal	802	802
Octane	802	800
2-Methyl pyrazine	825	831
2-Furanmethanol	861	865
1-(Acetyloxy)-2-propanone	871	867
Heptanal	902	901
Nonane	902	900
3-Methylthio propanal	906	905
2,3-Dimethyl pyrazine	919	918
Heptanol	971	967
Trimethyl pyrazine	1000	1012
Octanal	1002	1004
(2E)-Octenal	1058	1058
(2Z)-Nonenal	1094	1147
Nonanal	1105	1103
Octanoic acid	1175	1177
Decanal	1207	1205
(2E)-Decenal	1263	1259
Nonanoic acid	1271	1273
(2E, 4Z)-Decadienal	1296	1295
Undecanal	1308	1296
2-Undcenal	1364	1376
Decanoic acid	1367	1373
Dodecanal	1408	1398
β-Caryophyllene	1427	1422
Germacrene D	1487	1488
Tetradecanoic acid	1763	1760
9-Hexadecenoic acid	1946	1938
Hexadecanoic acid	1973	1970
(9Z)-Octadecanoic acid methyl ester	2094	2107
9-Octadecenoic acid	2142	2137
Octadecanoic acid	2163	2172

LRI exp= experimental linear retention index
LRI lit= experimental linear retention index, retrieved from database/literature.