

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

Selenia De Grazia^{1,2,¥}, Emanuela Gionfriddo^{1,¥} and Janusz Pawliszyn^{1*}

¹Department of Chemistry, University of Waterloo, Ontario, N2L 3G1, Canada

²Dipartimento di Scienze del Farmaco e dei Prodotti per la Salute (SCIFAR), University of Messina, Viale Annunziata, 98168 Messina, Italy

¥ Equal contribution of authors

Supporting Information

*Author to whom correspondence should be addressed: e-mail:

janusz@uwaterloo.ca, 200 University Avenue West, N2L 3G1 Waterloo, Ontario, Canada

De Grazia S., Gionfriddo E. and Pawliszyn J. - A new and efficient Solid Phase Microextraction approach for analysis of high fat content food samples using a matrix-compatible coating

Figure captions

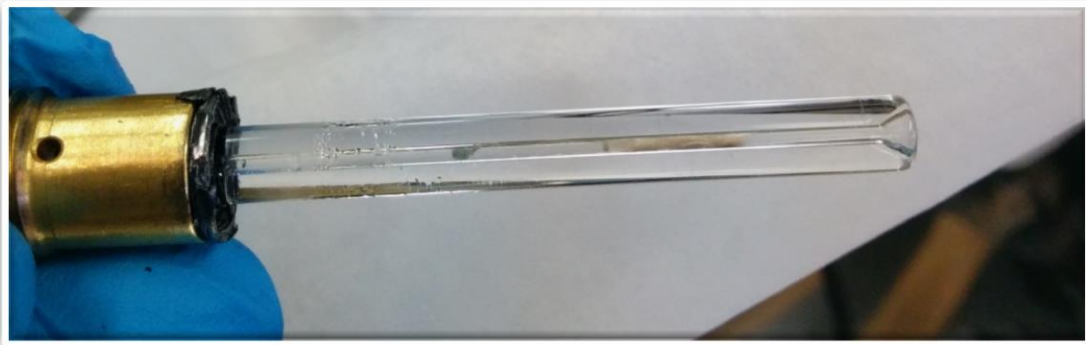
Figure S1. Glass liner of the 1079 Split/Splitless Injector contaminated by greasy, non-volatile compounds from avocado puree samples.

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).

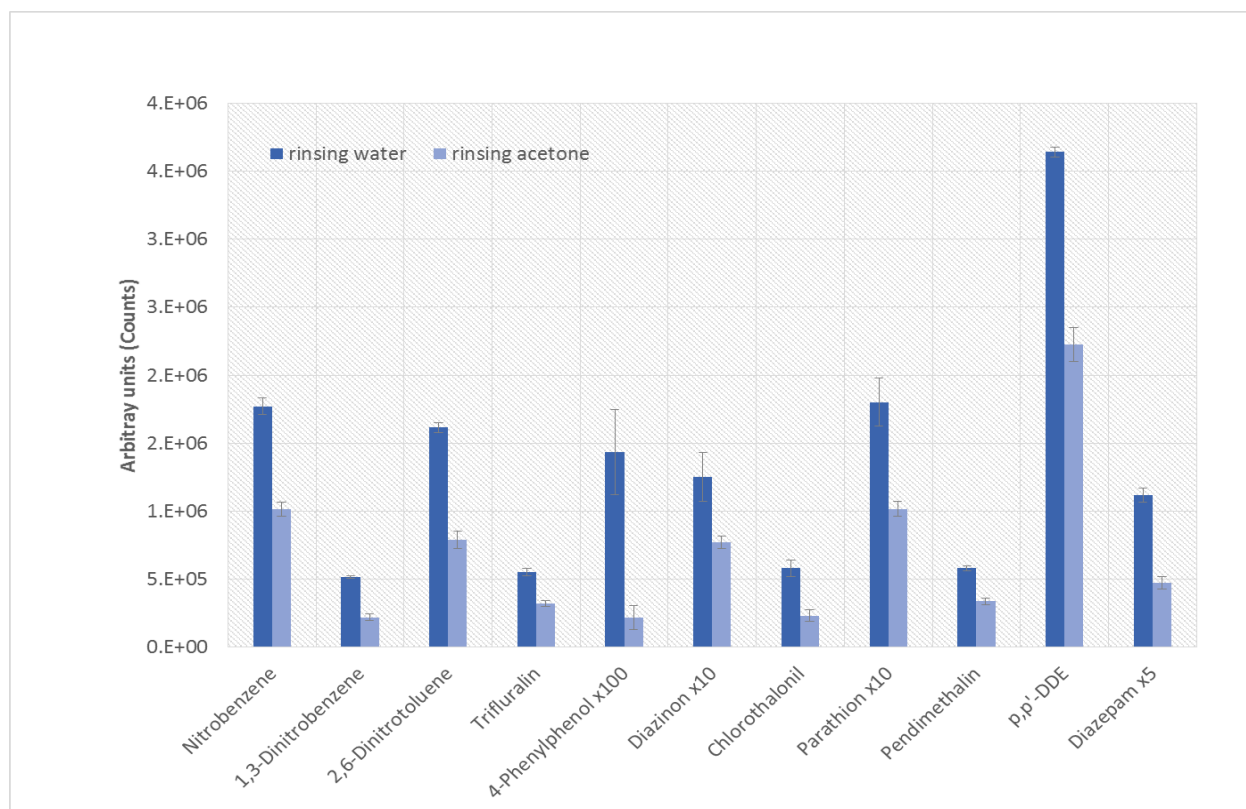
Figure S4: Response of QC analysis for PDMS/DVB/PDMS and PDMS/DVB used respectively for n=100 and n=50 extractions from avocado puree, before and after manual cleaning.

Figure S1



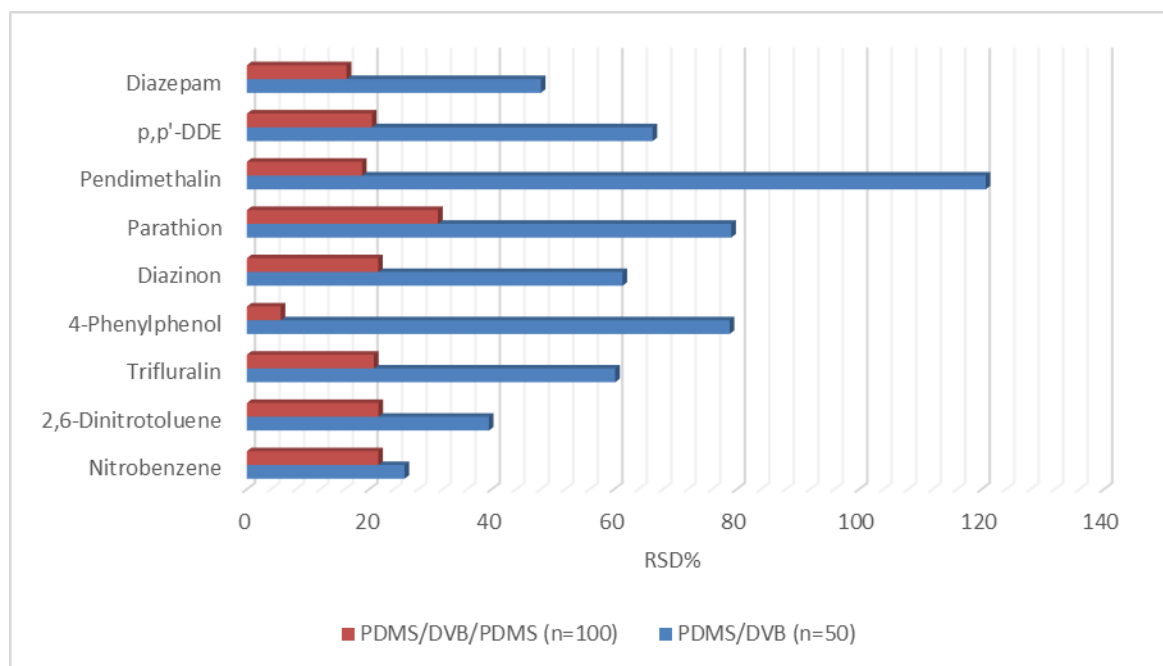
De Grazia S., Gionfriddo E. and Pawliszyn J. - A new and efficient Solid Phase Microextraction approach for analysis of high fat content food samples using a matrix-compatible coating

Figure S2



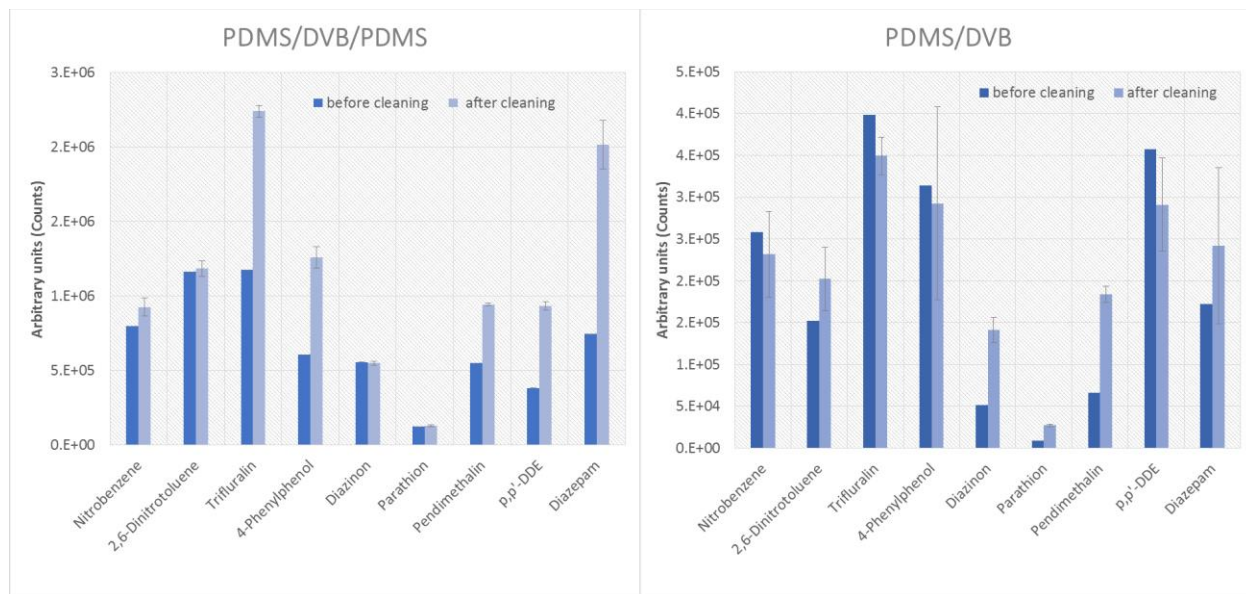
De Grazia S., Gionfriddo E. and Pawliszyn J. - A new and efficient Solid Phase Microextraction approach for analysis of high fat content food samples using a matrix-compatible coating

Figure S3



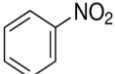
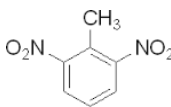
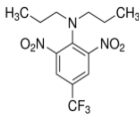
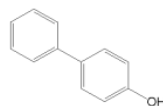
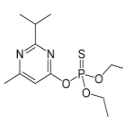
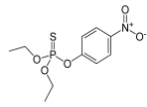
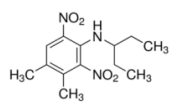
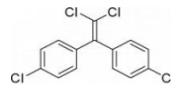
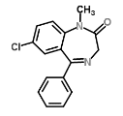
De Grazia S., Gionfriddo E. and Pawliszyn J. - A new and efficient Solid Phase Microextraction approach for analysis of high fat content food samples using a matrix-compatible coating

Figure S4



De Grazia S., Gionfriddo E. and Pawliszyn J. - A new and efficient Solid Phase Microextraction approach for analysis of high fat content food samples using a matrix-compatible coating

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

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

De Grazia S., Gionfriddo E. and Pawliszyn J. - A new and efficient Solid Phase Microextraction approach for analysis of high fat content food samples using a matrix-compatible coating

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

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

LRI exp= experimental linear retention index

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

De Grazia S., Gionfriddo E. and Pawliszyn J. - A new and efficient Solid Phase Microextraction approach for analysis of high fat content food samples using a matrix-compatible coating