

Characterization and quantification of microplastics and organic pollutants in mussels by microwave-assisted sample preparation and analytical pyrolysis

SUPPLEMENTARY MATERIAL

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Table S.1- List of the masses and m/z ions used for the SIM acquisition.

	Contaminant	MW	m/z used for SIM acquisition
PCB	2,4,4'-Trichlorobiphenyl (PCB28)	256	256
	2,2',5,5'-Tetrachlorobiphenyl (PCB52)	290	292
	2,2',4,5,5'-Pentachlorobiphenyl (PCB101)	324	326
	2,2',3,4,4',5'-Hexachlorobiphenyl (PCB138)	358	360
	2,2',4,4',5,5'-Hexachlorobiphenyl (PCB153)	358	360
	2,2',3,4,4',5,5'-Heptachlorobiphenyl (PCB180)	392	394
	Decachlorobiphenyl (PCB209)	494	498
PAH	naphthalene	128	128
	acenaphthylene	152	152
	acenaphthene	152	152
	fluorene	166	166
	phenanthrene	178	178
	anthracene	178	178
	fluoranthene	202	202
	pyrene	202	202
	benz(a)anthracene	228	228
	chrysene	228	228
	benzo(b)fluoranthene	252	252

	benzo(k)fluoranthene	252	252
	benzo(a)pyrene	252	252
	dibenz[a,h]anthracene	278	278
	benzo[g,h,i]perylene	276	276
	indeno[1,2,3-C,D]pyrene	276	276
CEC	methiocarb	225	168
	diclofenac	295	214
	3-tert-butyl-4-hydroxyanisole	180	165
	2-ethylhexyl 4-methoxycinnamate	290	178
PAE	dibutyl phthalate	278	149
	benzyl butyl phthalate	312	149
	bis (2-ethylhexyl) phthalate	390	149
	bis(7-methyloctyl) phthalate	418	149
	bis(8-methylnonyl) phthalate	446	149

Table S.2- Pyrolysis products and m/z quantification ions used for the quantitative analysis of microplastics.

Polymer	Pyrolysis product used for quantification	m/z quantification ion
PE	α,ω -alkenes C ₁₅ -C ₂₅ (average of the areas)	82
PP	2,4-dimethyl-1-heptene	126
PS	3-butene-1,3- diylidibenzene (styrene dimer)	91
ABS	2-phenethyl-4- phenylpent-4-enitrile (SAS)	170
SBR	butadiene trimer	79
PMMA	methyl methacrylate (MMA)	100
PC	bisphenol A (BPA)	213
PVC	naphthalene	128
PET	benzoic acid (BA)	122
N6	caprolactam	133
N66	cyclopentanone	84

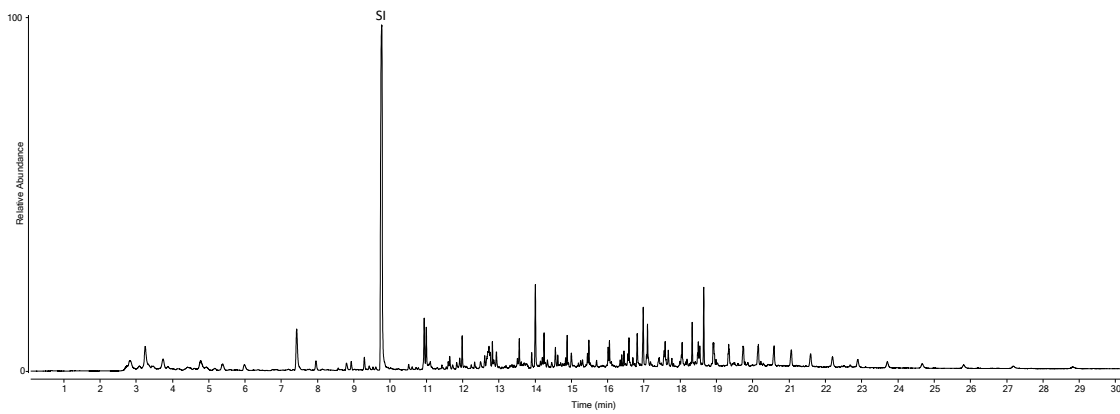


Figure S.1- Total ion chromatogram of the Py-GC-MS analysis of the filter with the particles after the digestion with HCl.

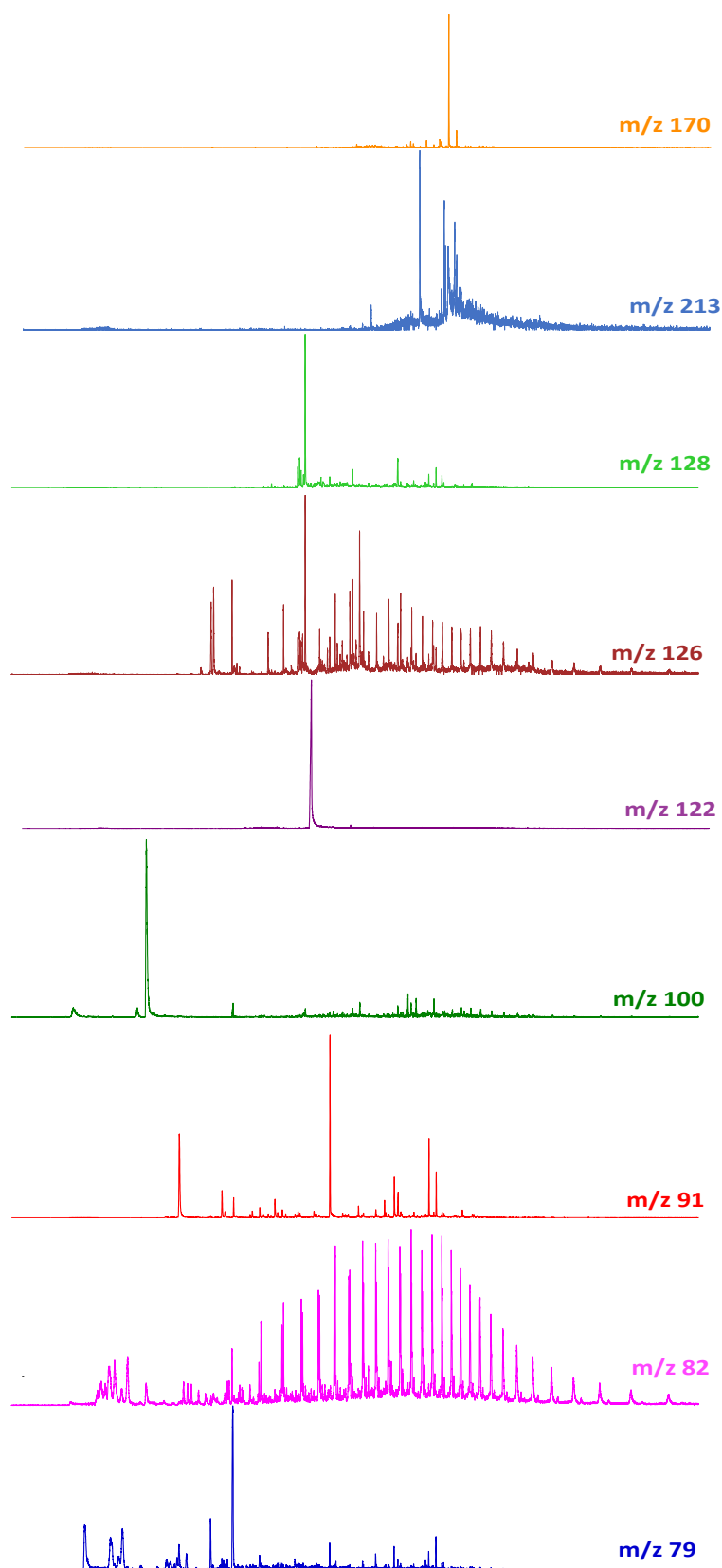


Figure S.2- Extracted ion chromatograms of the TIC reported in Figure S.1, using the m/z characteristic of the polymers: m/z 79 for SBR, 82 for PE, 91 for PS, 100 for PMMA, 122 for PET, 126 for PP, 128 for PVC, 213 for PC, and 170 for ABS.