Release of selected non-intentionally added substances (NIAS) from PET food contact materials: a new online SPE -UHPLC-MS/MS multiresidue method.

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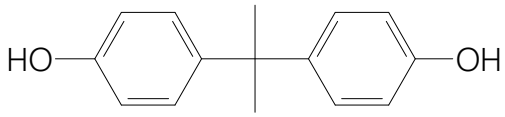
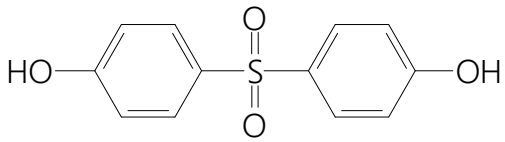
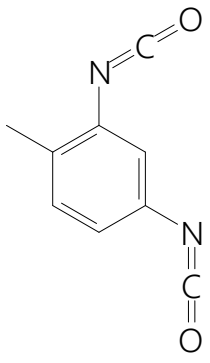
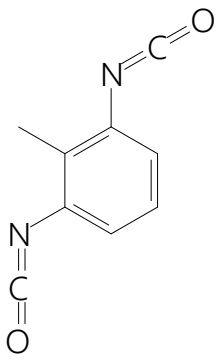
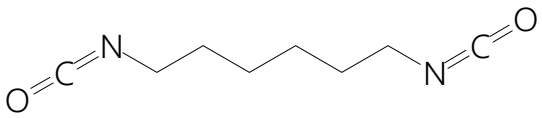
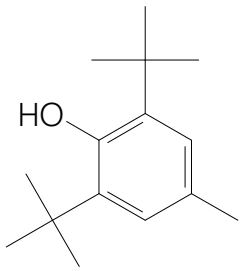
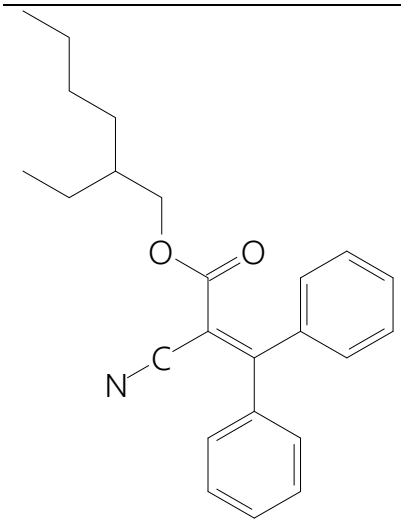
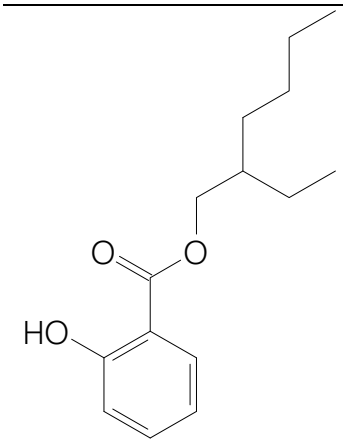
Supplementary materials

Structural formulae	**Name** **Abbreviation** **Molecular formulae** **Molecular weight**
	Bisphenol A BPA $C_{15}H_{16}O_2$ MW 228.29
	Bisphenol S BPS $C_{12}H_{10}O_4S$ MW 228.29
	Toluene-2,4-diisocyanate 2,4-TDI $C_9H_6N_2O_2$ MW 174.15

	Toluene-2,6-diisocyanate 2,4-TDI $C_9H_6N_2O_2$ MW 174.15
	hexamethylene diisocyanate HDI $C_8H_{12}N_2O_2$ MW 168.19
	2,6-di-tert-butyl-4-methylphenol BHT $C_{15}H_{24}O$ MW 220.35
	Octocrylene $C_{24}H_{27}NO_2$ MW 361.48
	2-ethylhexyl salicylate $C_{15}H_{22}O_3$ MW 250.33

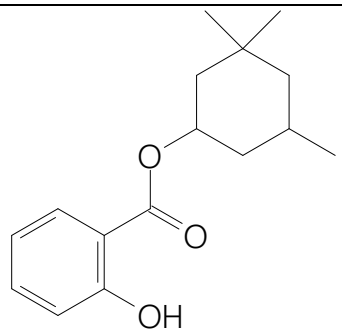
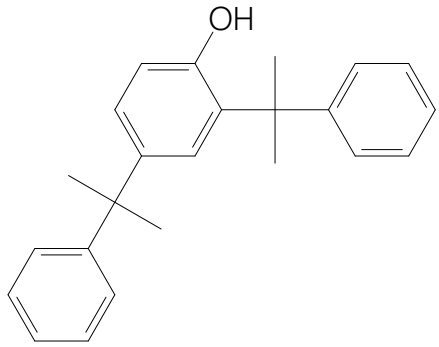
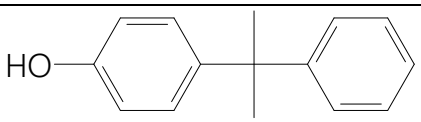
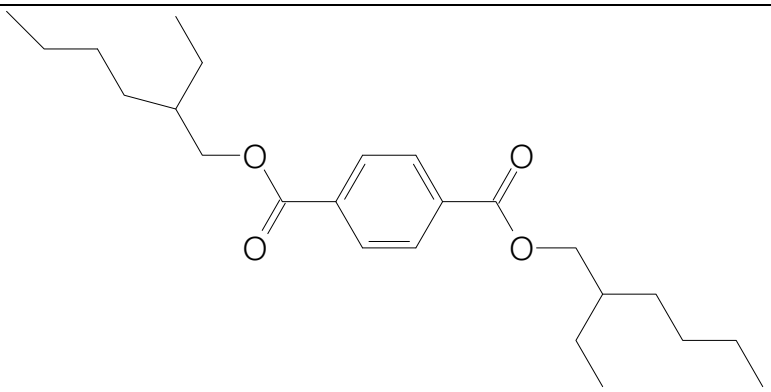
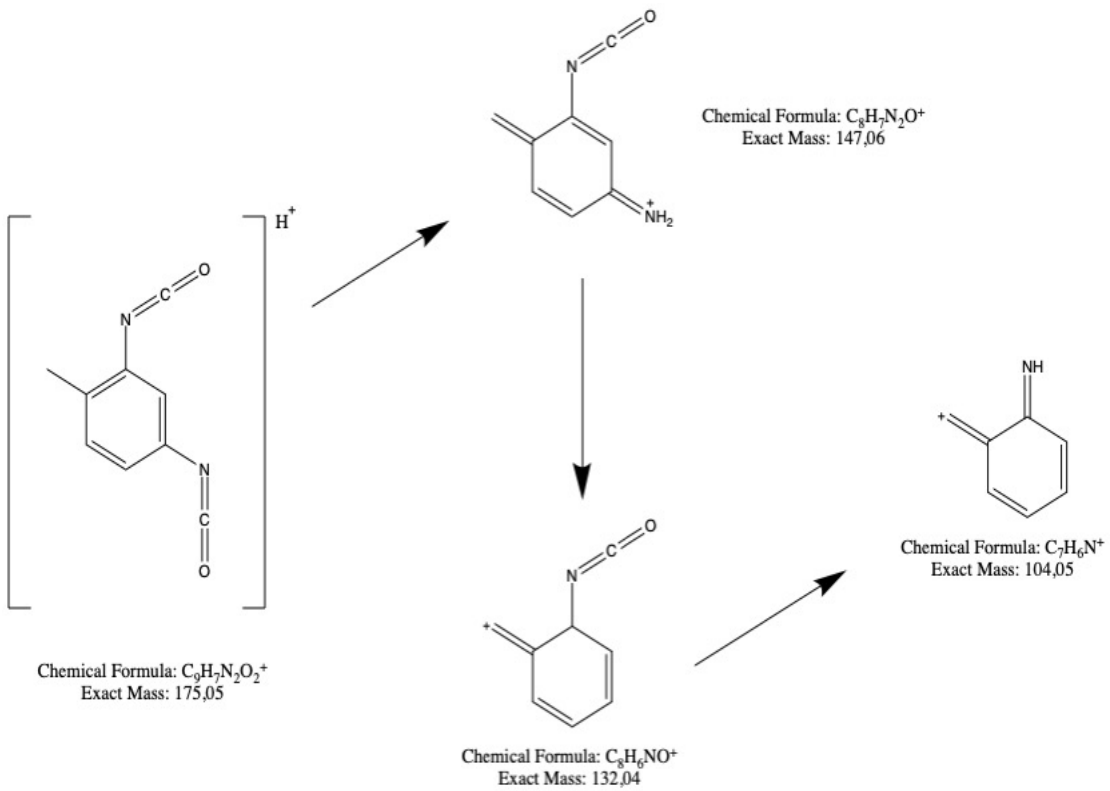
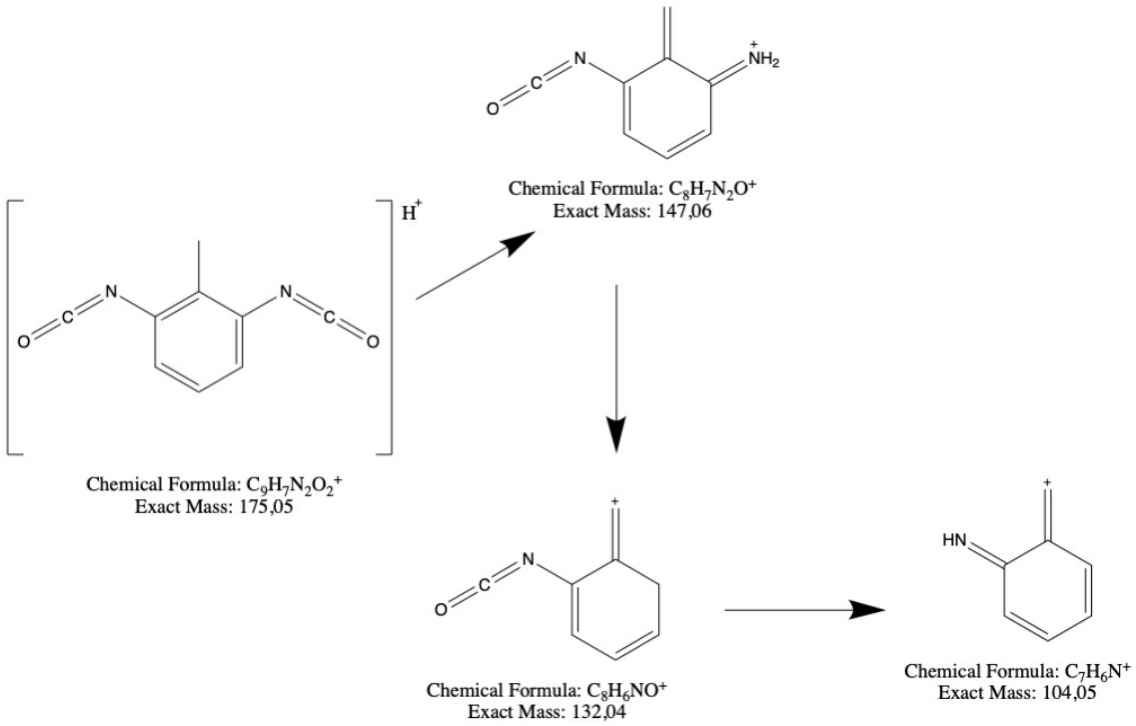
	Homosalate $C_{16}H_{22}O_3$ MW 262.34
	2,4-dicumylphenol $C_{24}H_{26}O$ MW 330.46
	4-cumylphenol $C_{15}H_{16}O$ MW 212.29
	bis(2-ethylhexyl) terephthalate BEHT $C_{24}H_{38}O_4$ MW 390.56

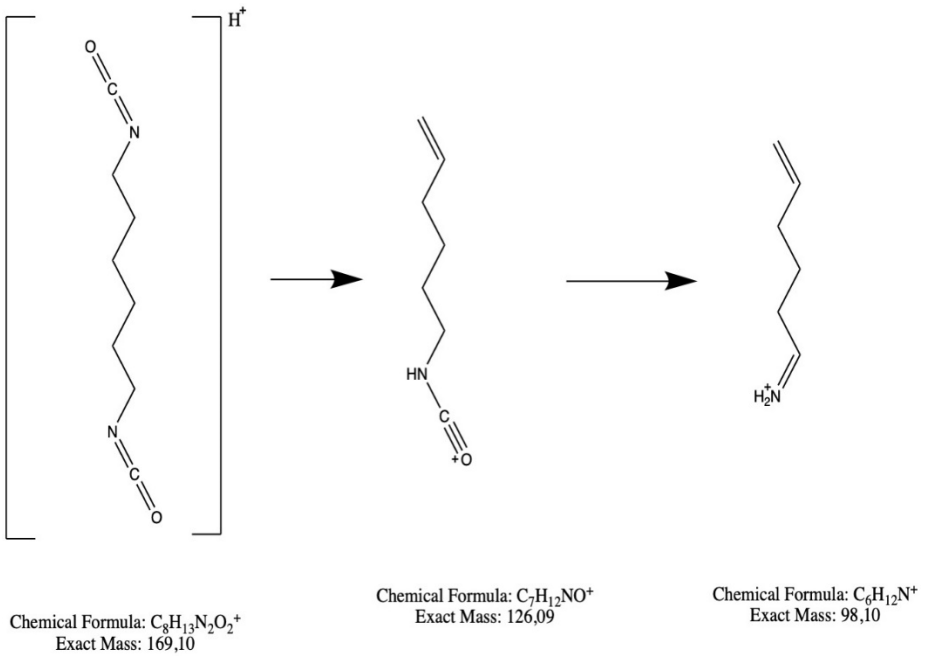
Figure S1: structural formulae, name, abbreviation, molecular formulae and molecular weight of the selected analytes



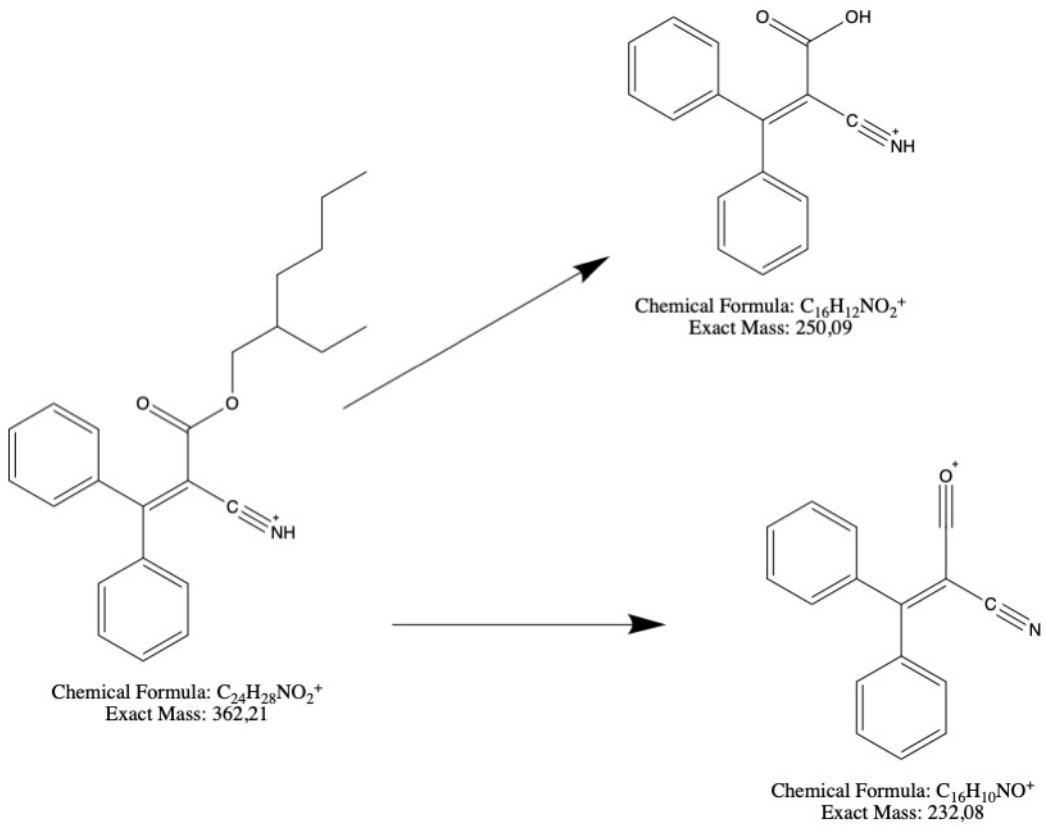
Scheme S1: fragmentation pathway of 2,4-TDI (ESI positive).



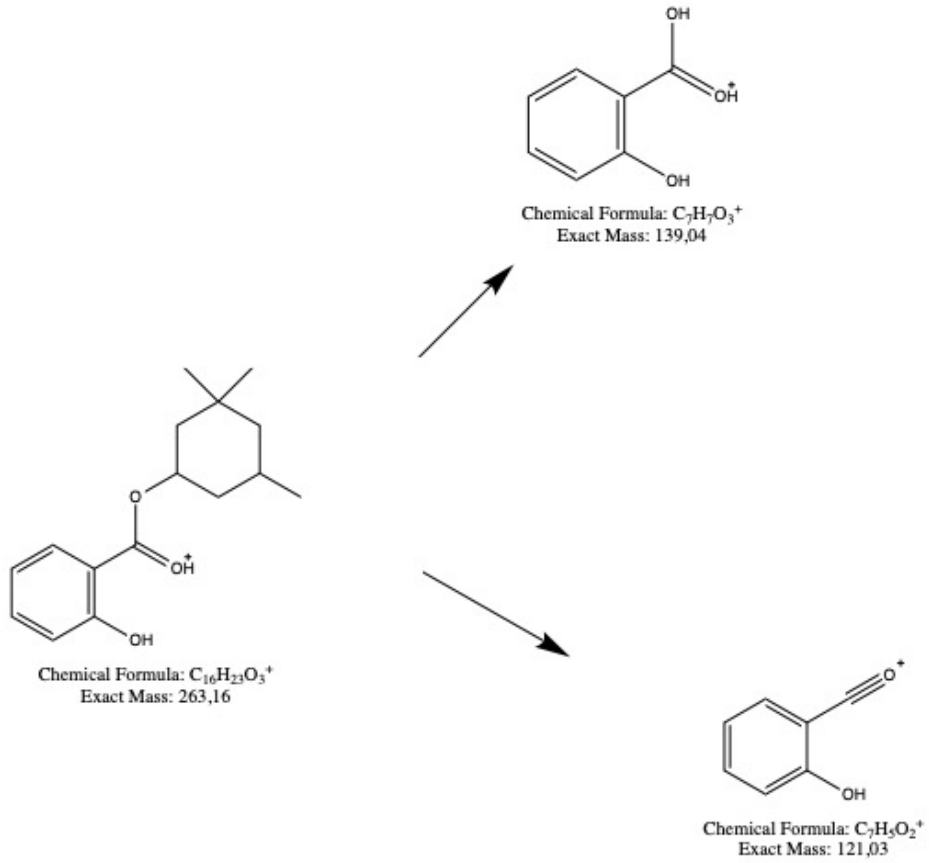
Scheme S2: fragmentation pathway of 2,6-TDI (ESI positive).



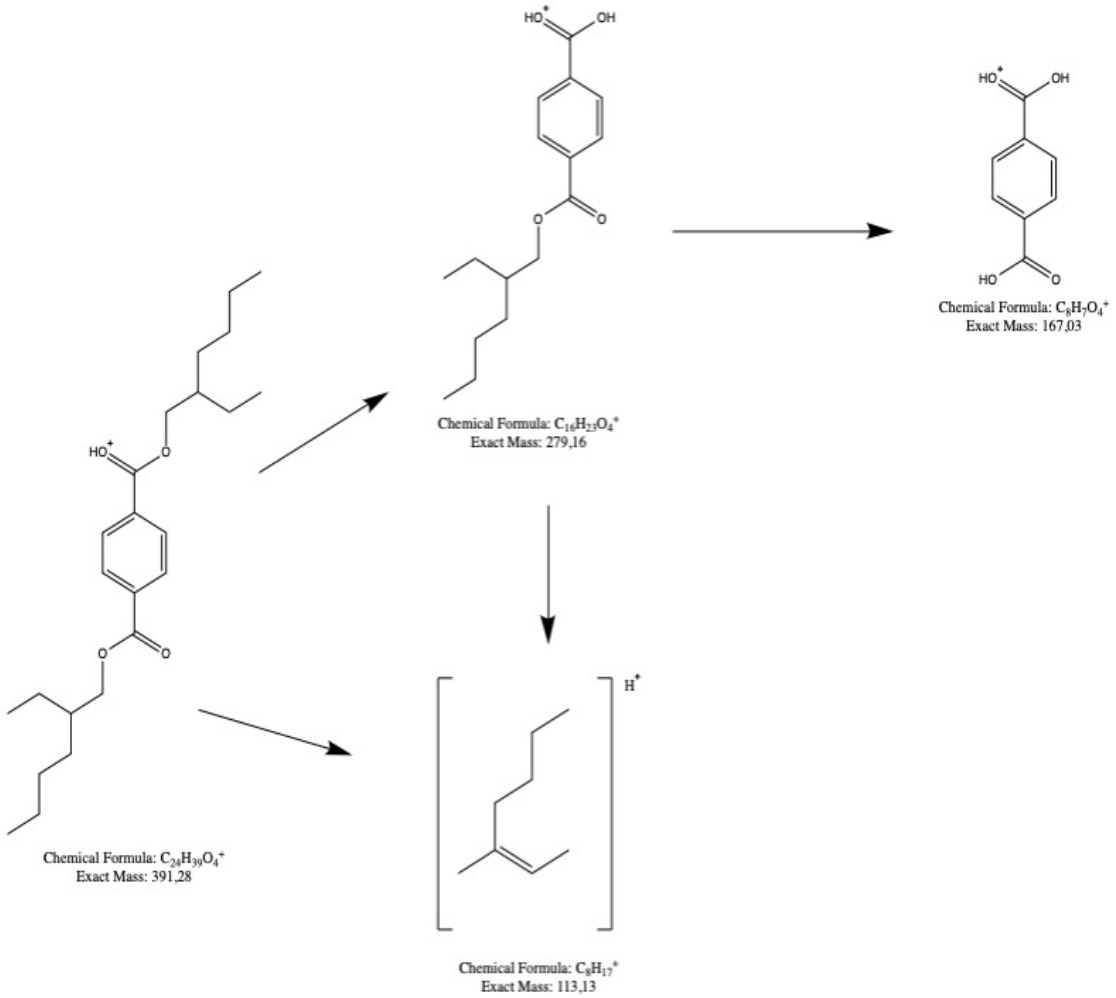
Scheme S3: fragmentation pathway of HDI (ESI positive).



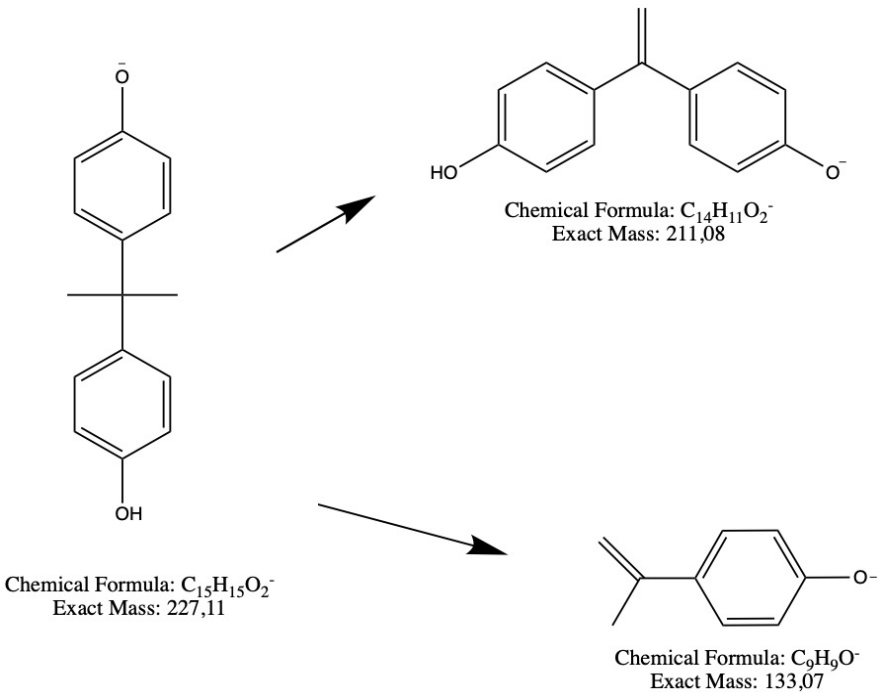
Scheme S4: fragmentation pathway of octocrylene (ESI positive).



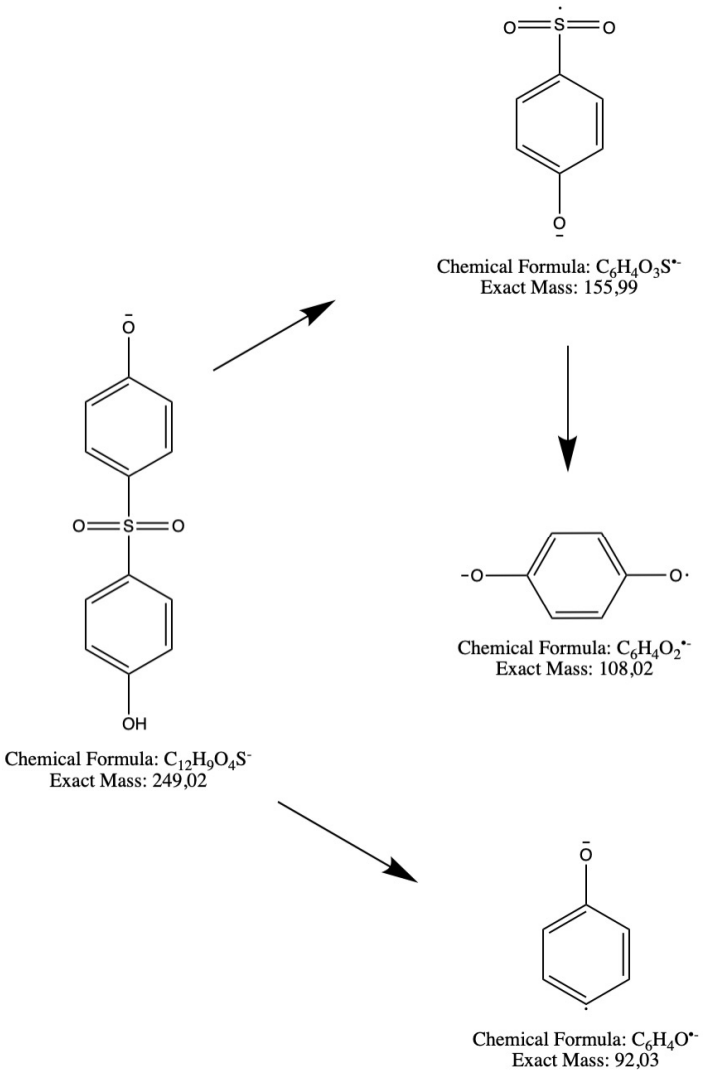
Scheme S5: fragmentation pathway of homosalate (ESI positive).



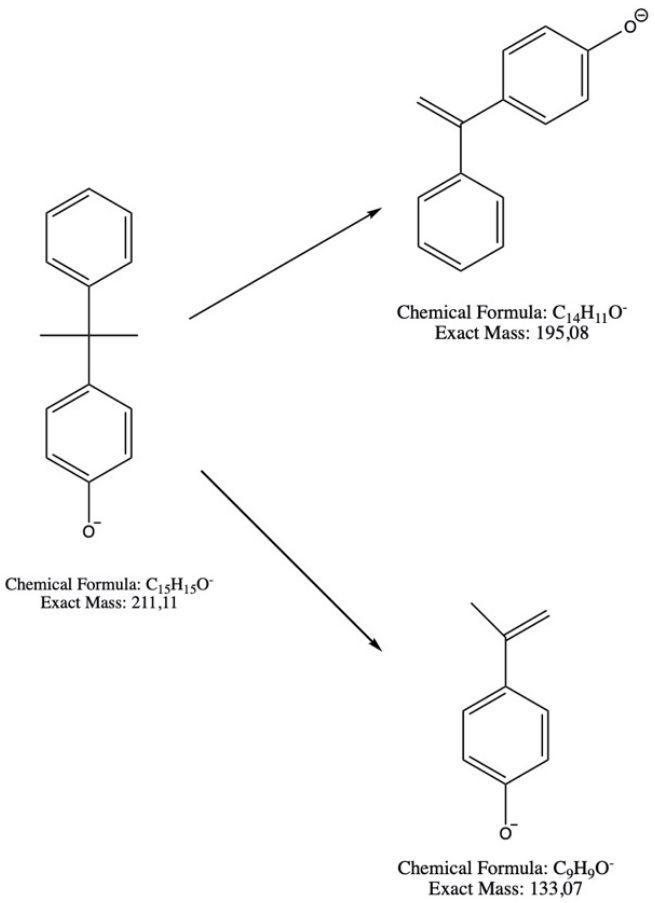
Scheme S6: fragmentation pathway of BEHT (ESI positive).



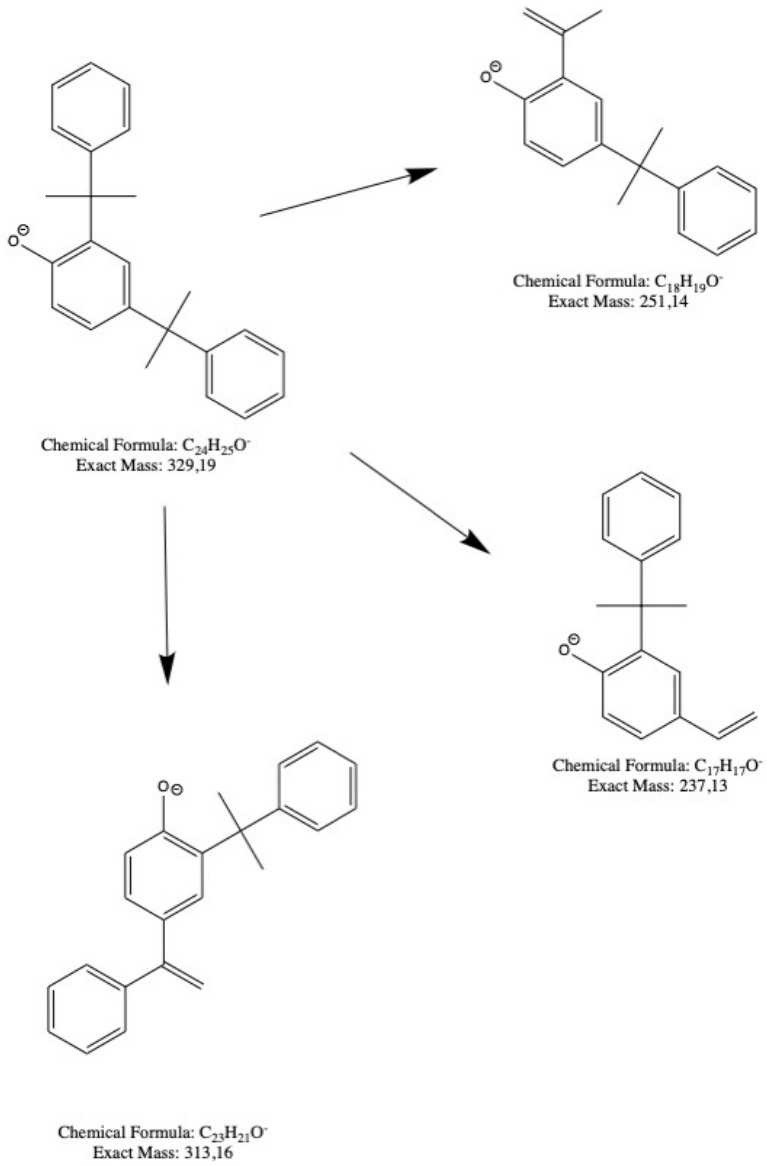
Scheme S7: fragmentation pathway of BPA (ESI negative).



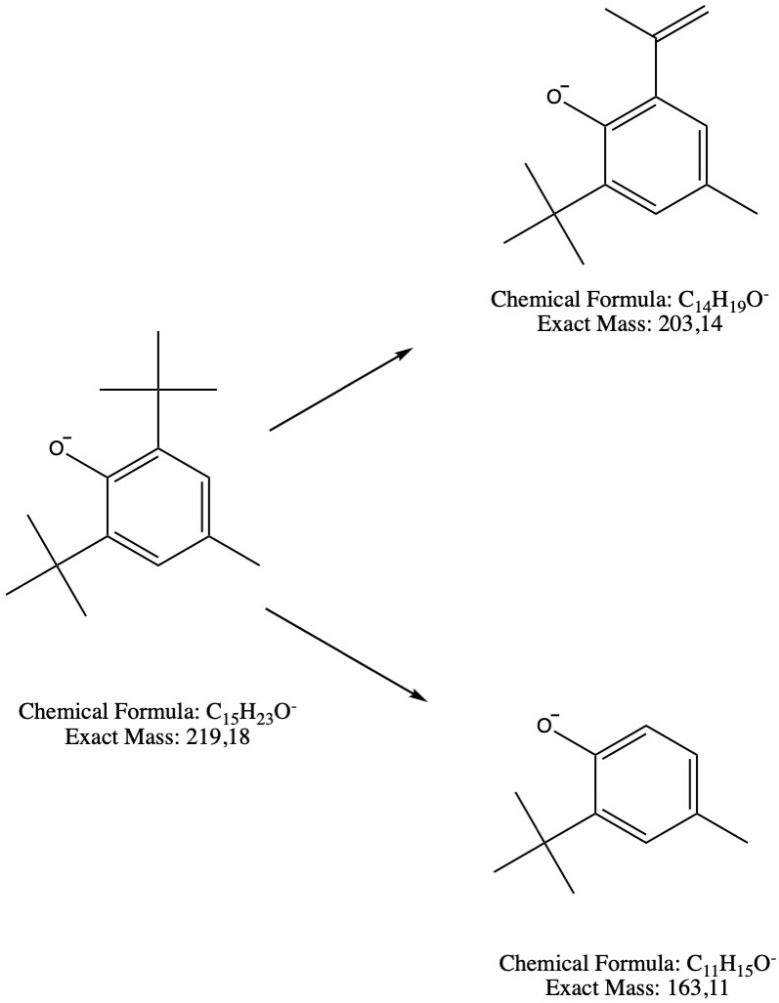
Scheme S8: fragmentation pathway of BPS (ESI negative).



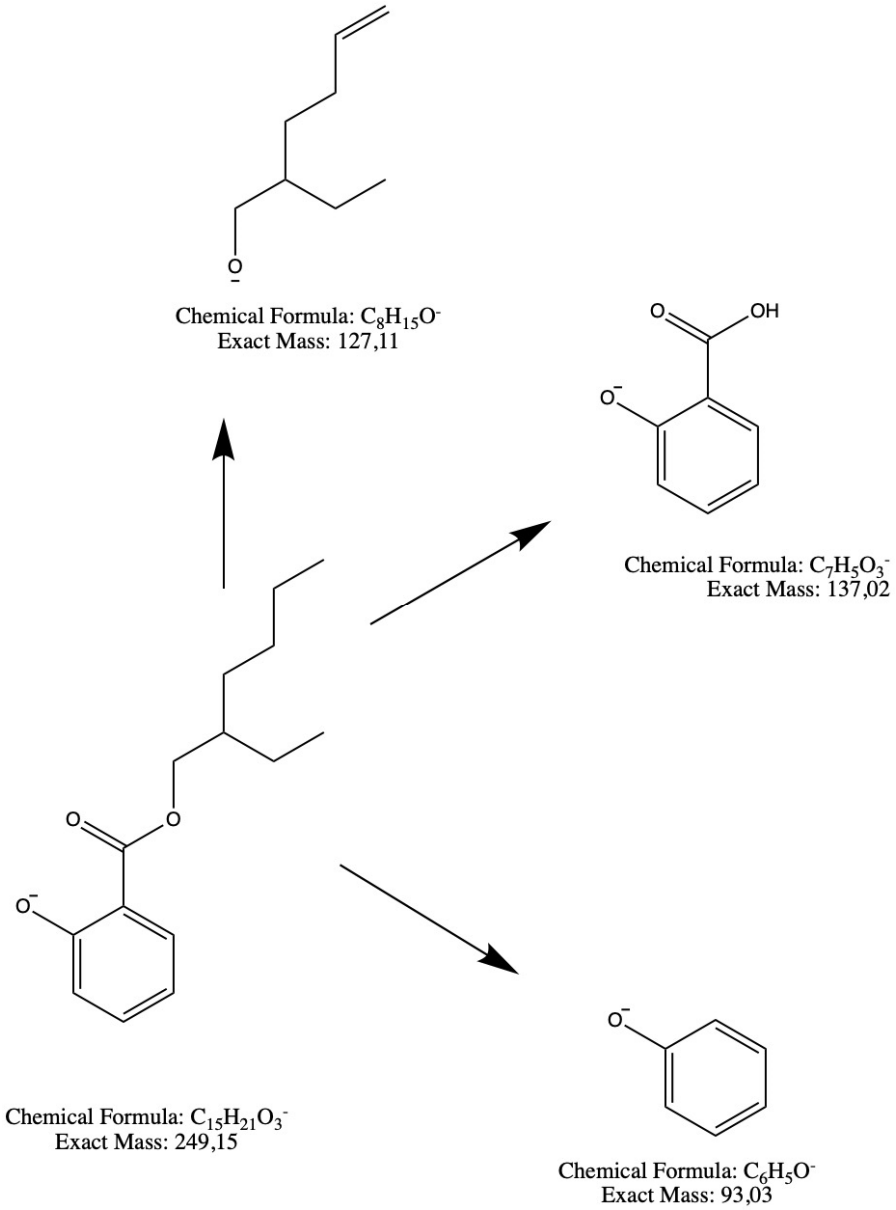
Scheme S9: fragmentation pathway of 4-cumylphenol (ESI negative).



Scheme S10: fragmentation pathway of 2,4-dicumylphenol (ESI negative).



Scheme S11: fragmentation pathway of BHT (ESI negative).



Scheme S12: fragmentation pathway of 2-ethylhexyl salicylate (ESI negative).