Supplementary material to:

Transformation products of the high-volume production chemicals 1-vinyl-2-pyrrolidinone and 2-piperazin-1-ylethanamine formed by UV photolysis

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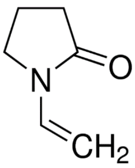
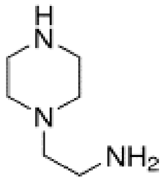
Table S1. VP and PPE properties and structure.

Compound Name	1-vinylpyrrolidin-2-one	2-piperazin-1-ylethanamine
Acronym	VP	PPE
CAS Number	88-12-0	140-31-8
Molecular formula	C_6H_9NO	$C_6H_{15}N_3$
Log D (pH 7.4) [(1)]	0.38	-4.53
Log P [(1)]	0.37	-0.86
Boiling point (760 mmHg) [(1)]	217 ºC	220ºC
Consumer uses [(2)]	Washing and cleaning products, cosmetics and personal care products, paints, coatings, and adhesives. Laboratory chemicals.	Adhesives, sealants, coatings, paints. pH regulators and water treatment products.
Harmonised classification and labelling (CLP00) [(2)]	GHS05 Corrosive, GHS06 Acute toxicity, GHS09 Hazardous to the environment	GHS05 Corrosive, GHS07 Health hazard
Structure		

[(1)] Predicted values, ACDLabs, [(2)] Data from www.echa.europe.eu

Table S2. Photochemical kinetic parameters obtained from non-linear fitting to an exponential decay and calculation of quantum yields (UPW: ultrapure water; SW: surface water).

	k (min^{-1}) [a]	**$t_{1/2}$ (min) [a]**	**R^2**	**ε (M^{-1} cm^{-1})**	**Φ (mol/einstein) [a]**
VP (UPW)	0.36 ± 0.03	1.9 ± 0.2	0.9989	$4.38 \cdot 10^3$	0.28 ± 0.03
VP (SW)	0.33 ± 0.01	1.7 ± 0.1	0.9999	-	-
PPE (UPW)	0.017 ± 0.001	40 ± 3	0.9728	3.66	16 ± 1
PPE (SW)	0.019 ± 0.002	36 ± 3	0.9908	-	-
DCF (UPW)	0.50 ± 0.06	1.4 ± 0.2	0.996	$5.76 \cdot 10^3$	0.292 [b]

[a] Mean ± 95% confidence interval

[b] Value from (Wols et al., 2012)

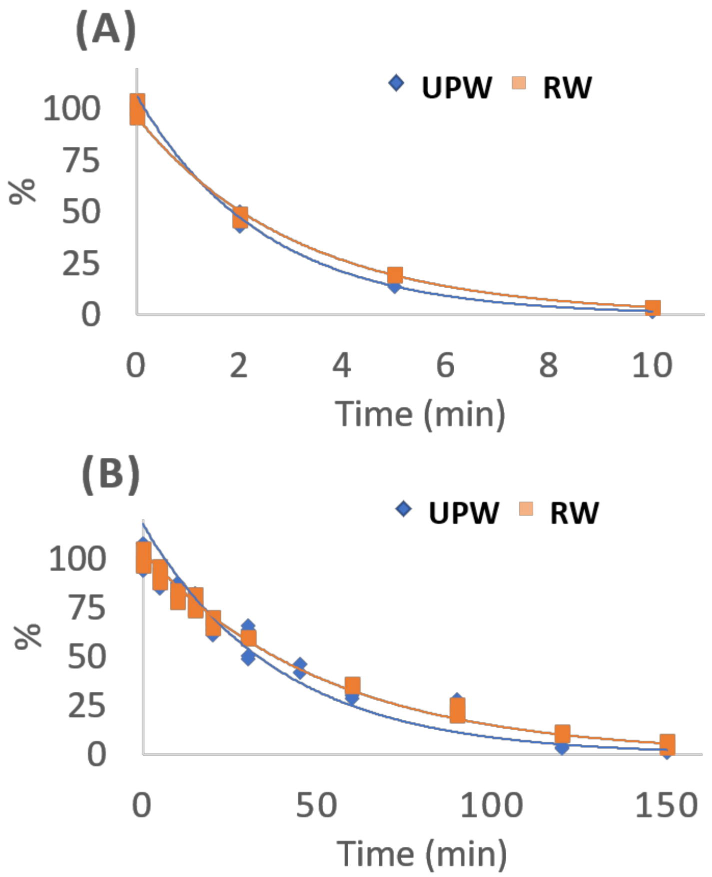


Figure S1. UV photolysis kinetic plots in ultrapure (UPW) and river water (RW) of (A) VP and (B) PPE. Data normalized to time 0 (untreated samples).

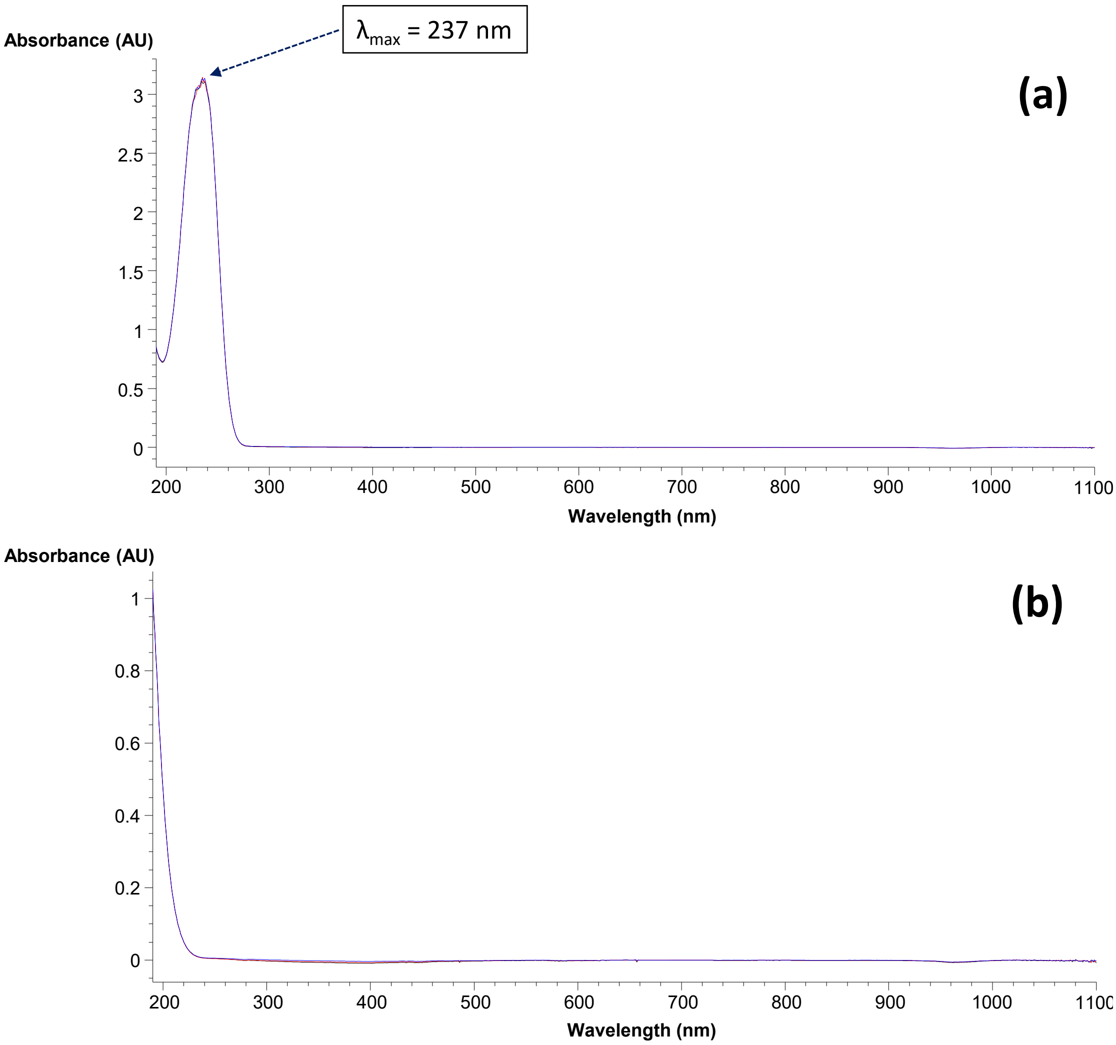


Figure S2: UV/Vis absorption spectrum of (a) VP and (b) PPE.

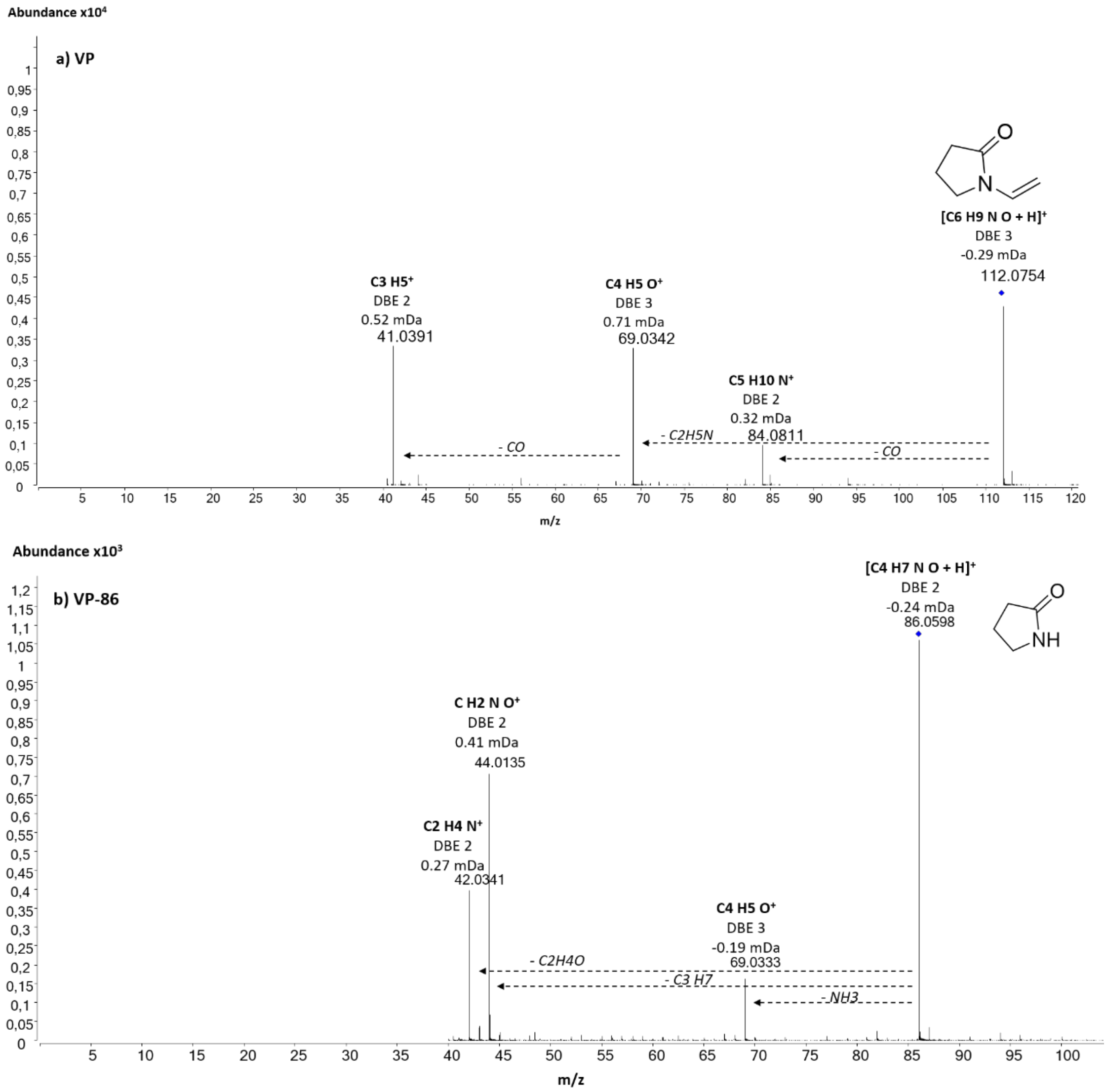


Figure S3. QTOF product ion spectra of VP and its TPs. (a) VP and (b) VP-86

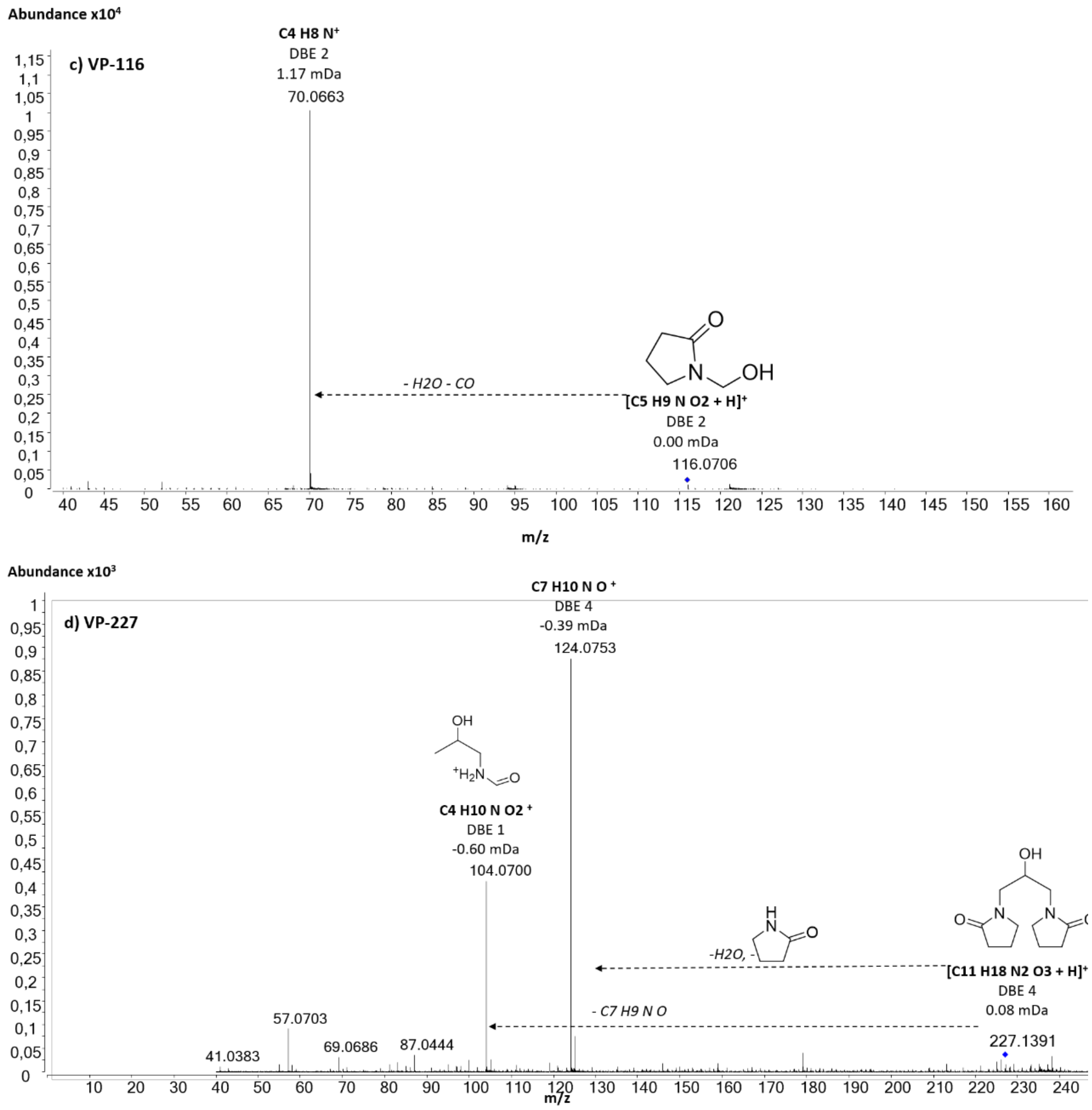


Figure S3 cont. QTOF product ion spectra of VP and its TPs. (c) VP-116 and (d) VP-227

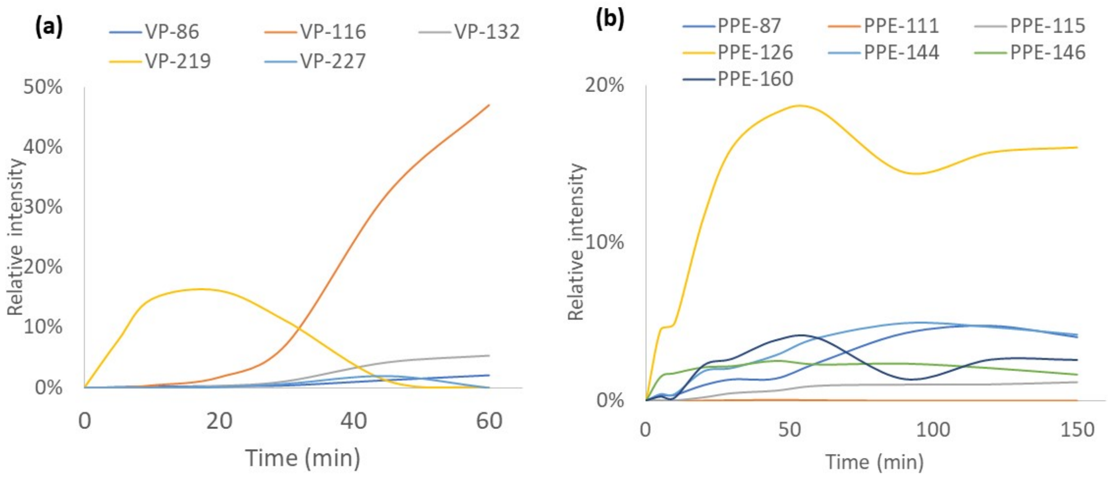


Figure S4. TPs formation profiles for VP (a) and PPE (b). Signal of TPs normalized to the signal of their parent chemical at time 0.

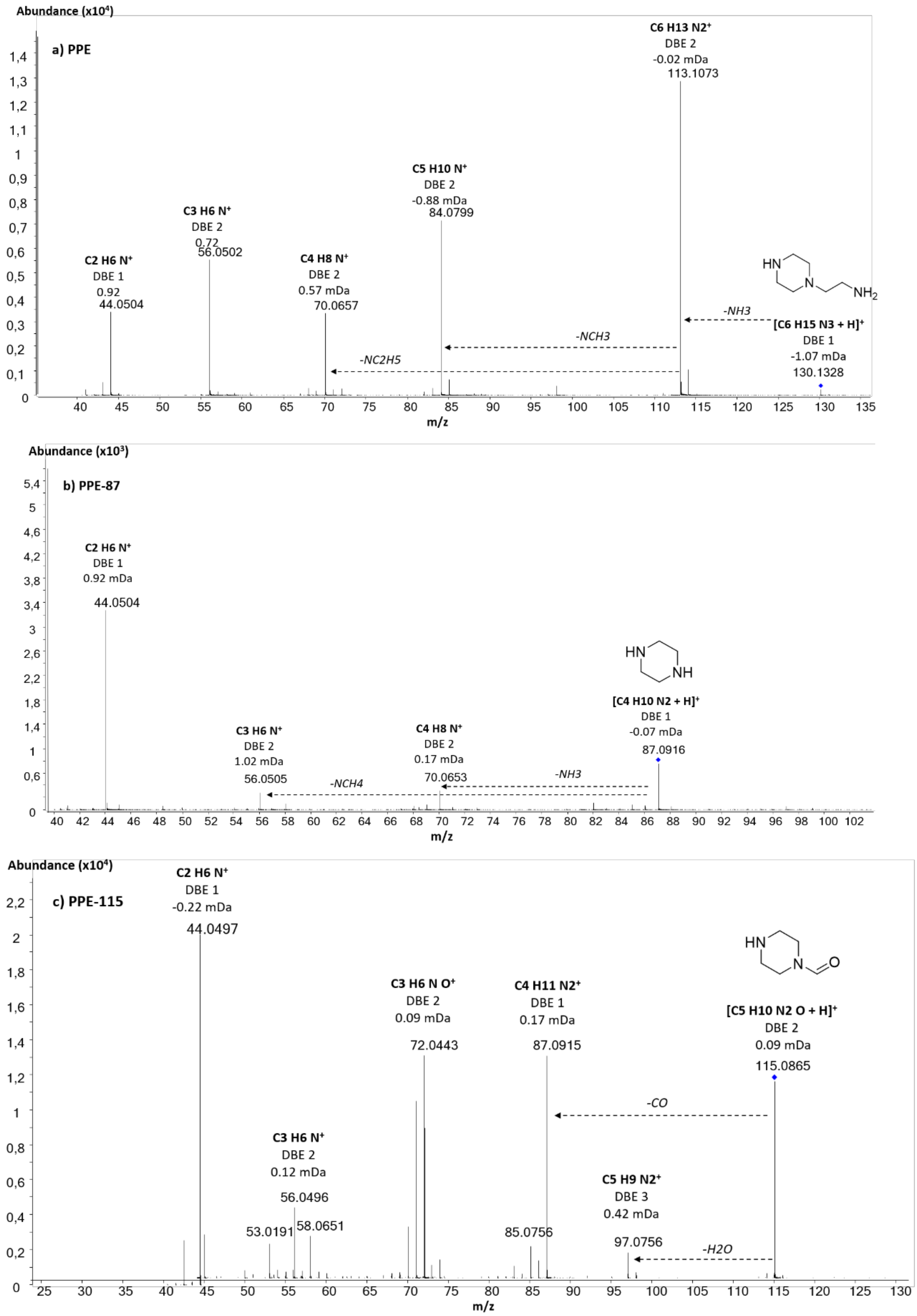


Figure S5: QTOF product ion spectra of PPE and its TPs. (a) PPE , (b) PPE-87 and (c) PPE-115

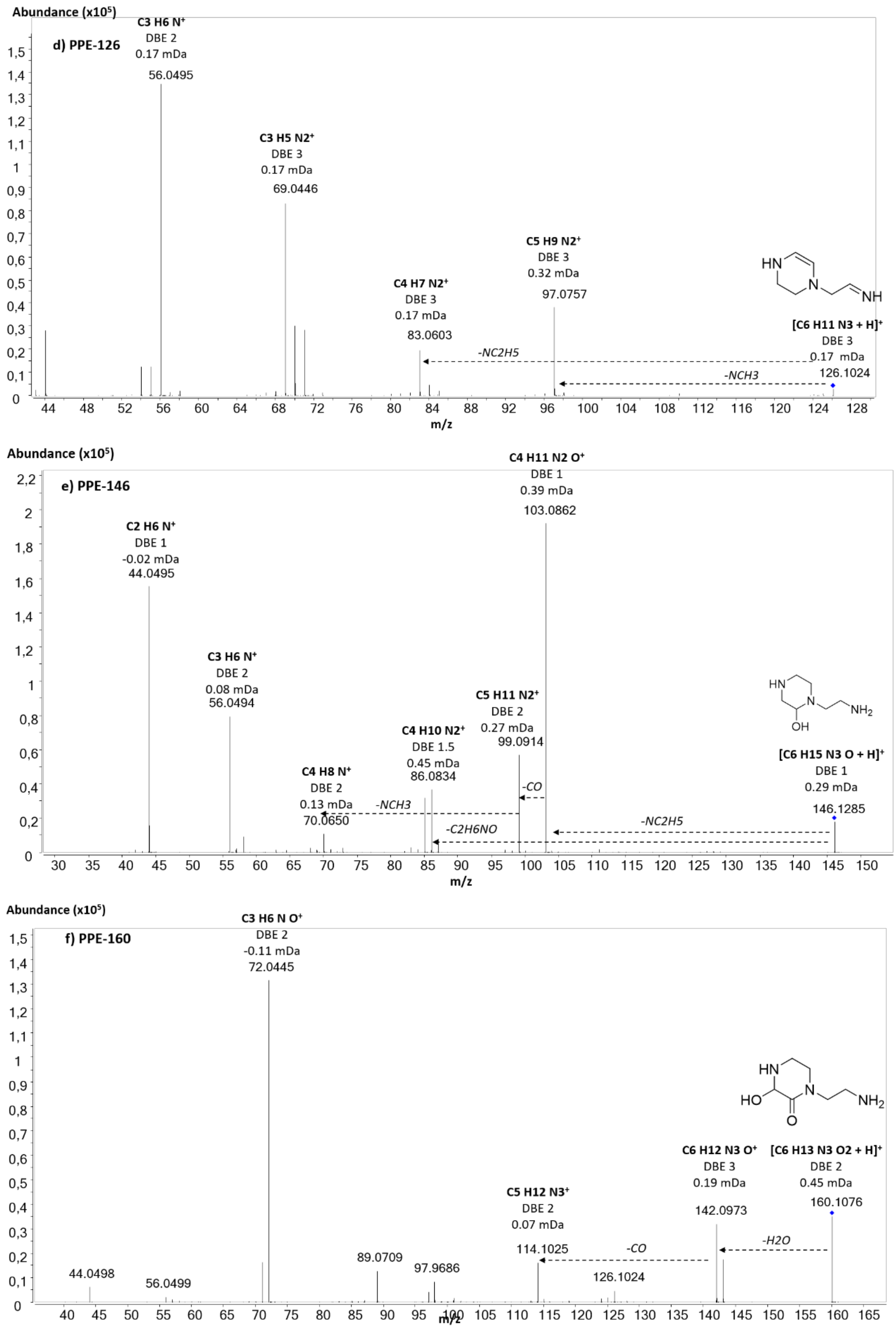


Figure S5 cont: QTOF product ion spectra of PPE and its TPs. (d) PPE-126, (e) PPE-146 and (f) PPE-160

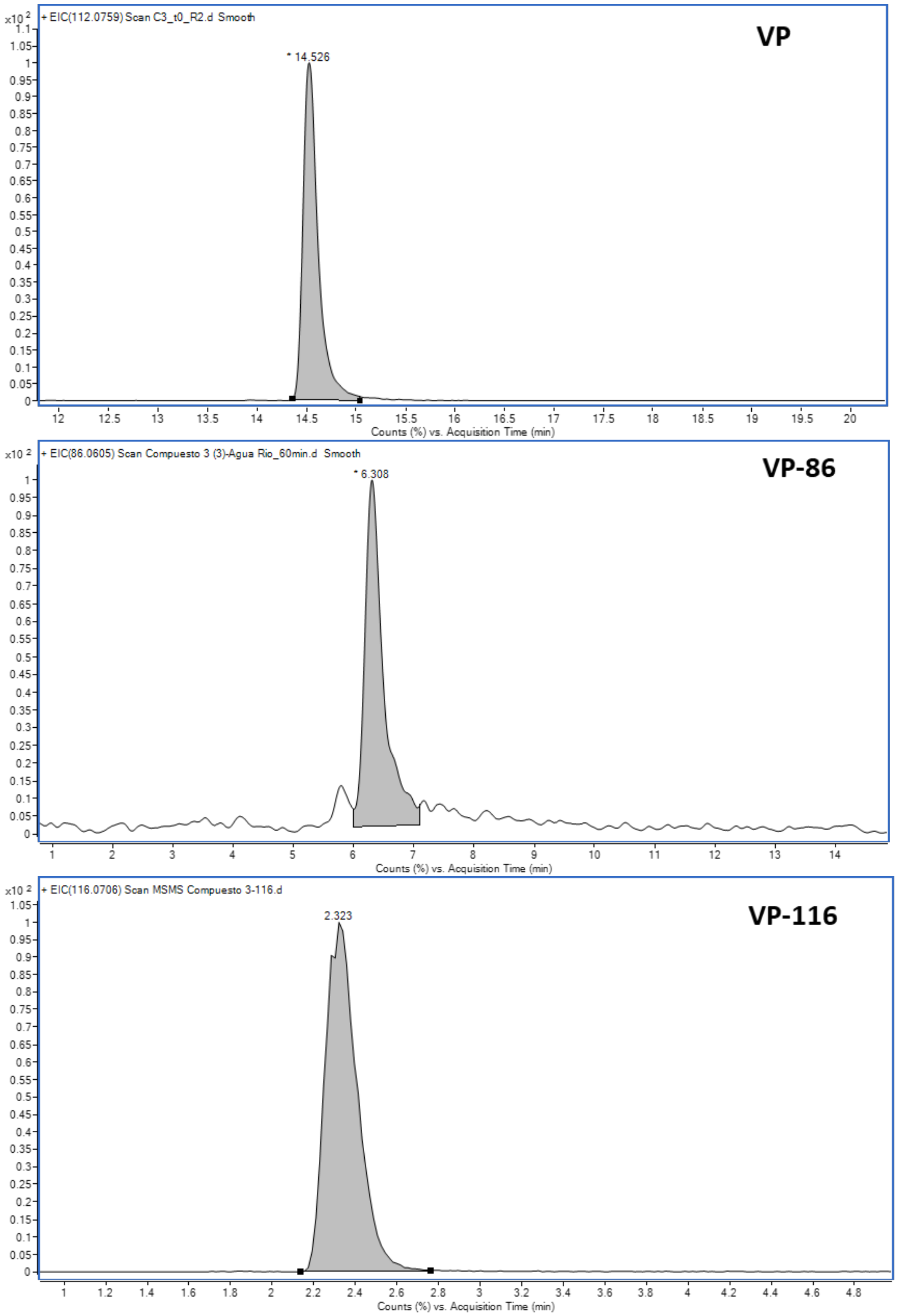


Figure S6: Extracted ion chromatograms of VP and identified TP

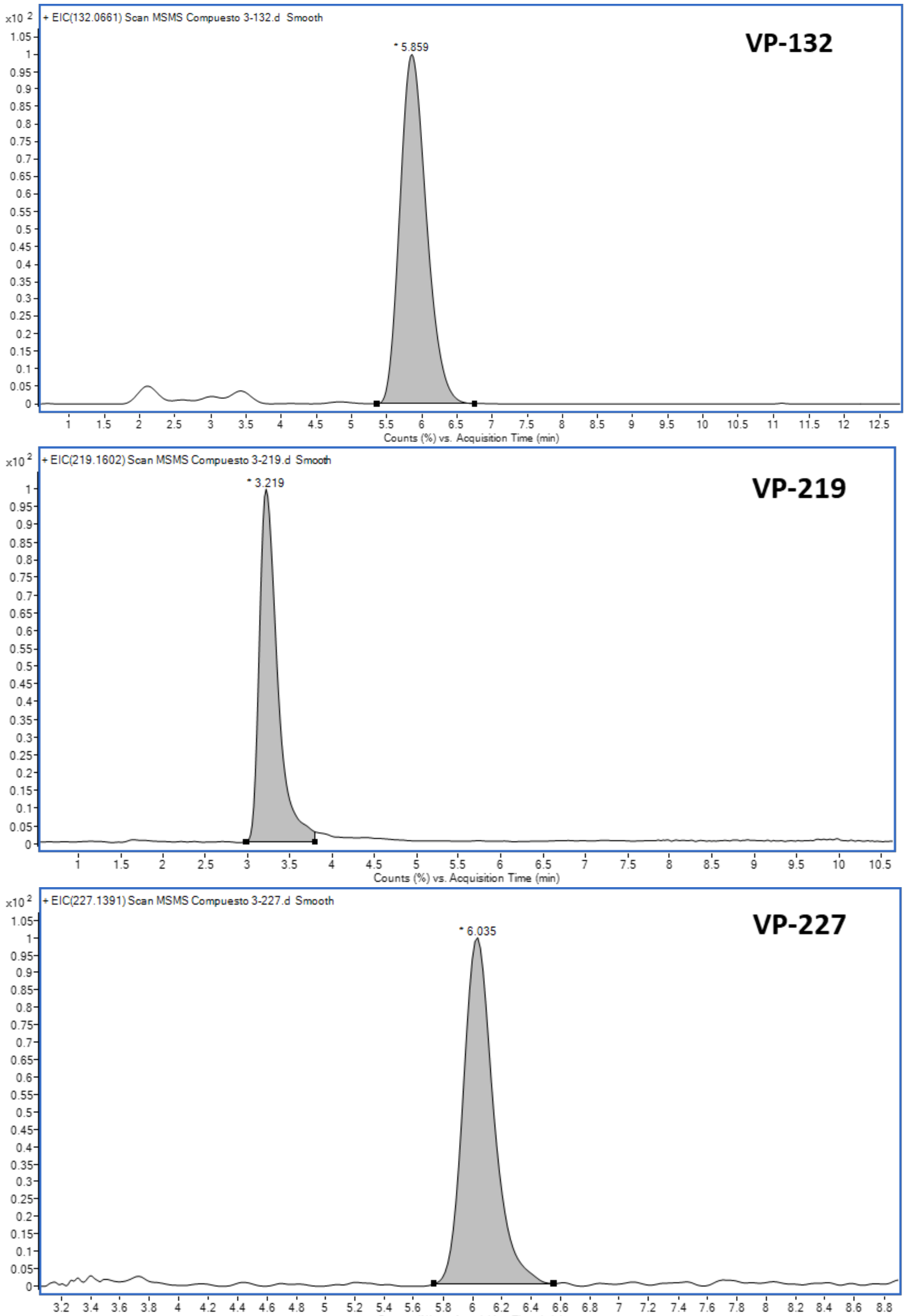


Figure S6 cont: Extracted ion chromatograms of VP identified TP

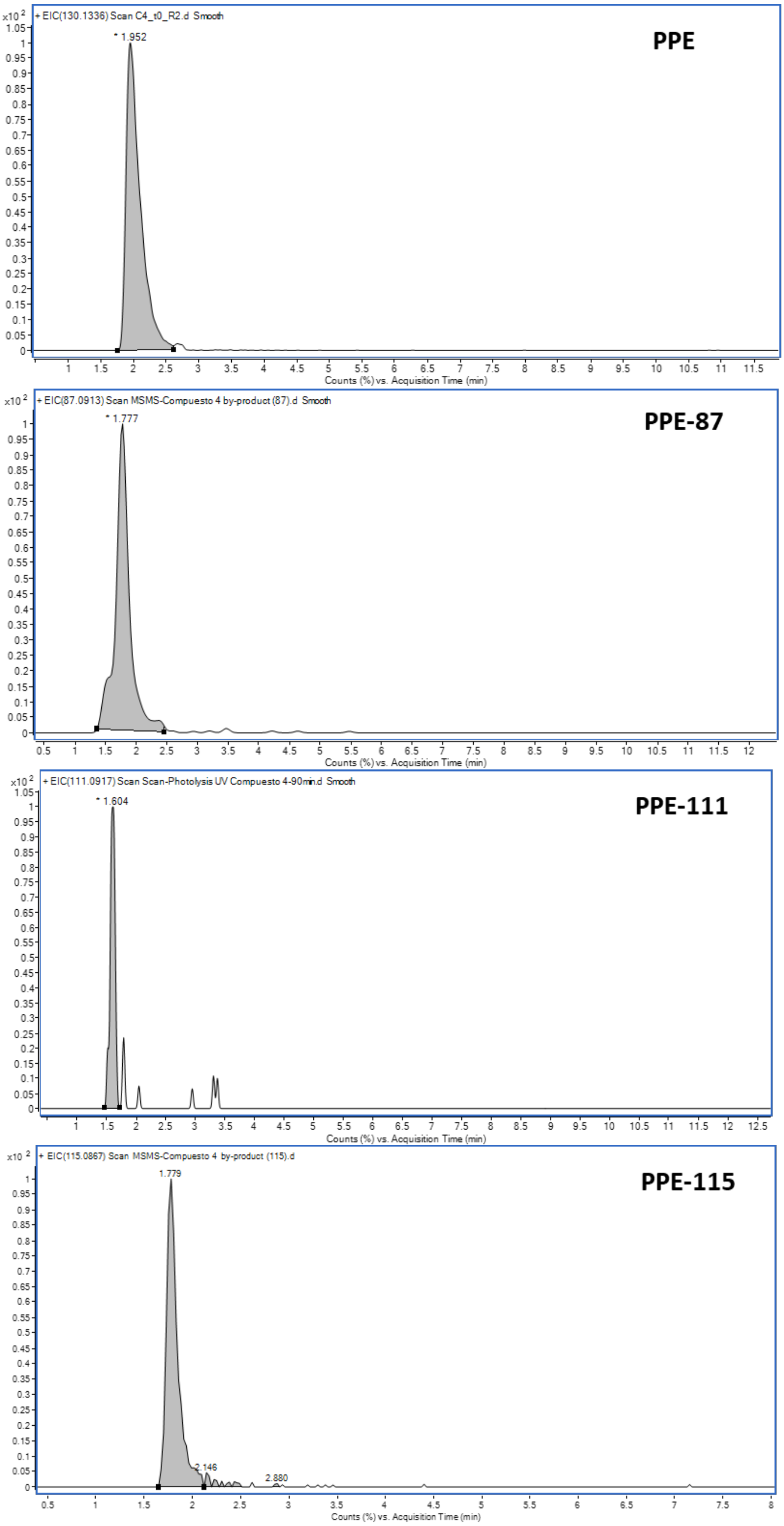


Fig S7: Extracted ion chromatograms of PPE and identified TP

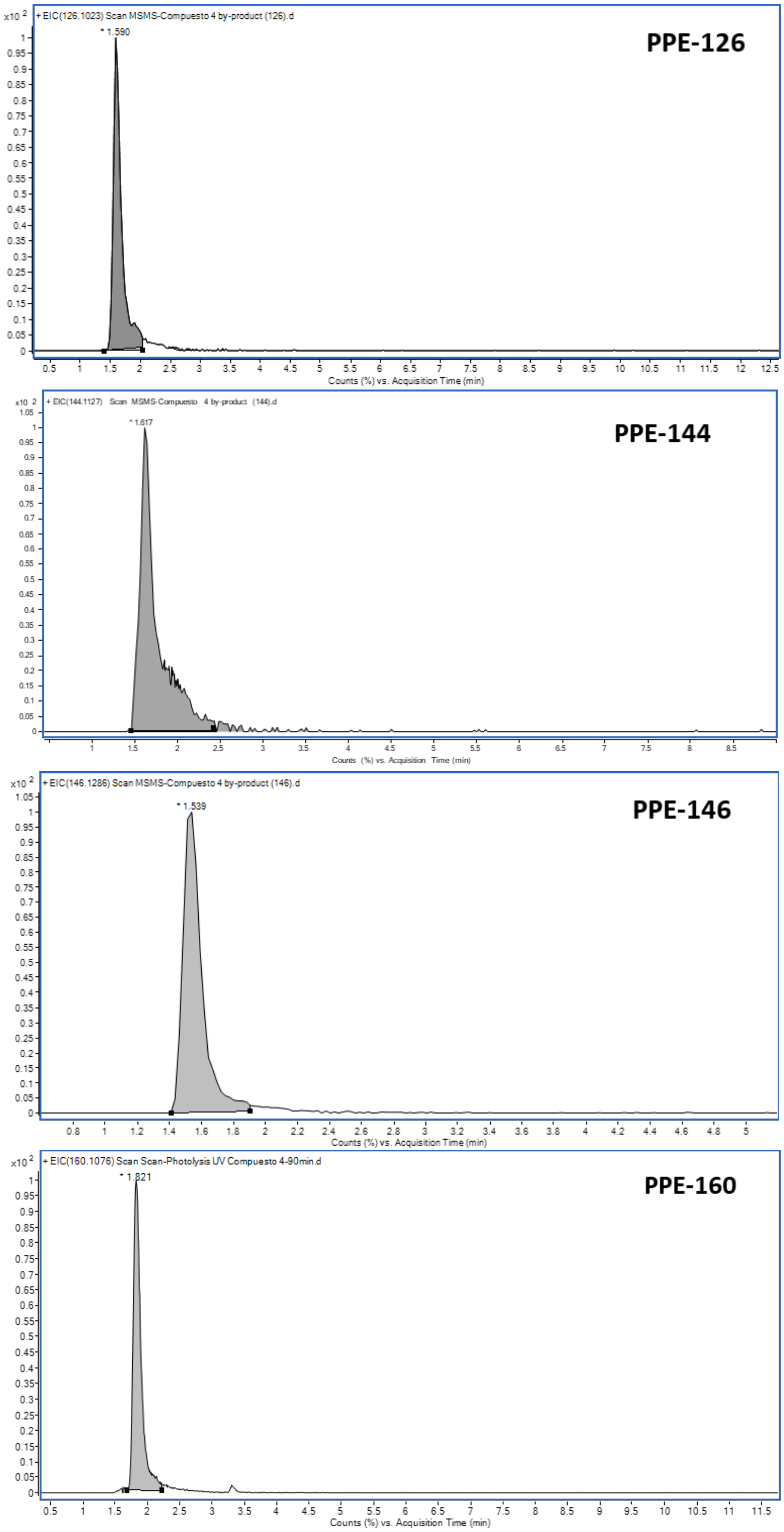


Fig S7 cont.: Extracted ion chromatograms of PPE identified TP

Table S3. Summary of EPA T.E.S.T. predicted toxicity endpoints. Note: n.a. means that no prediction was possible.

Compound	***Fathead minnow***	***Daphnia magna***	***T. pyrifromis***	**Oral rat**
	LC_{50} 96 h mg/L	**LC_{50} 48 h mg/L**	**IGC_{50} 48 h mg/L**	**LD_{50} mg/Kg**
VP	1.73E+02	1.36E+01	1.62E+03	1.36E+03
VP-86	4.86E+02	4.17E+01	3.14E+03	1.11E+03
VP-116	1.39E+03	1.15E+02	7.42E+03	1.16E+03
VP-132	2.49E+03	3.61E+02	8.92E+03	8.92E+03
VP-219	1.09E+02	2.83E+00	n.a.	7.37E+02
VP-227	1.91E+02	4.32E+02	1.53E+03	4.71E+03
PPE	2.55E+03	6.07E+01	1.59E+03	1.78E+03
PPE-87	1.37E+03	1.31E+02	2.02E+03	2.09E+03
PPE-111	9.06E+02	4.43E+01	4.27E+02	1.29E+03
PPE-115	1.07E+03	2.15E+03	n.a.	1.80E+03
PPE-126	n.a.	n.a.	n.a.	n.a.
PPE-144	2.91E+03	6.96E+01	1.30E+03	2.75E+03
PPE-146	3.38E+03	2.11E+02	2.07E+03	3.37E+03
PPE-160	3.81E+03	4.10E+02	3.88E+03	3.23E+03

Table S4. Summary of ECOSAR predicted toxicity endpoints. Note: in some cases two values were obtained for the same TP, the (*) symbol is used when the estimation is based on the "amide" group class, while the other value was obtained when "aliphatic amine" group class was used.

	Acute toxicity			**Chronic toxicity**		
Compound	**Fish 96h LC_{50}**	**Daphnid 48 h LC_{50}**	**Green Algae 96 h EC_{50}**	**Fish ChV**	**Daphnid ChV**	**Green Algae ChV**
*VP**	7.23E+02	9.16E+02	4.63E+01	4.38E+00	7.96E+01	1.36E+01
VP-86	1.53E+03	2.11E+03	7.98E+01	7.22E+00	1.49E+02	1.83E+01
VP-116	1.97E+04	3.29E+04	6.50E+02	5.36E+01	1.46E+03	8.57E+01
VP-132	3.40E+04	5.88E+04	1.03E+03	8.37E+01	2.40E+03	1.23E+02
VP-219	8.50E+01	9.60E+00	8.82E+00	5.84E+00	7.48E-01	2.82E+00
VP-227	4.08E+04	6.85E+04	1.33E+03	1.10E+02	3.01E+03	1.73E+02
PPE	5.48E+03	4.31E+02	8.09E+02	1.13E+03	2.37E+01	1.99E+02
PPE-87	1.14E+03	9.83E+01	1.54E+02	1.79E+02	5.89E+00	4.05E+01
PPE-111	2.63E+02	2.58E+01	3.13E+01	2.76E+01	1.76E+00	9.03E+00
PPE-115	4.79E+03	3.77E+02	7.06E+02	9.84E+02	2.07E+01	1.74E+02
PPE-115*	1.91E+04	3.19E+04	6.34E+02	5.24E+01	1.43E+03	8.40E+01
PPE-126	1.05E+03	9.39E+01	1.38E+02	1.49E+02	5.82E+00	3.71E+01
PPE-144	1.54E+04	1.13E+03	2.44E+03	3.94E+03	5.78E+01	5.70E+02
PPE-144*	7.34E+04	1.35E+05	1.94E+03	1.53E+02	4.78E+03	1.95E+02
PPE-146	6.31E+04	4.16E+03	1.11E+04	2.24E+04	1.92E+02	2.40E+03
PPE-160	1.75E+05	1.07E+04	3.31E+04	7.75E+04	4.62E+02	6.79E+03
PPE-160*	1.30E+06	2.99E+06	1.95E+04	1.37E+03	6.04E+04	9.96E+02