PET Flake Injection

Novel Technology Development

Data Monitoring Report

report required by Article 13 of Regulation (EU) 2022/1616

10 October 2023 amended 7th March 2024

(addition of Targeted analysis of inorganic substances by ICP-MS)

Also Results for Sample 9 have been withdrawn as it was established that the process used to produce the samples does not fit under the Flake injection Novel technology.

The data presented in this report are based on the measurements performed by a third-party laboratory, which was contracted by PET Europe. The data provided is the property of PET Europe and cannot be copied, reproduced, or distributed without their prior written consent. PET Europe are not responsible nor liable for any errors or inaccuracies that may have occurred during the measurement process by the third-party laboratory. The data are provided for informational purposes only and do not constitute any endorsement or recommendation by PET Europe.

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Introduction

The novel technology PET Flake Injection was notified as required under Articles 10(2) and 10(3) of Commission Regulation (EU) 2022/1616 on 17th March 2023.

Article 13 of Commission Regulation (EU) 2022/1616 States the following:

"a recycler operating a decontamination installation in accordance with Article 11 of the regulation shall monitor the average contaminant level on the basis of a robust sampling strategy which samples the plastic input batches and the corresponding plastic output batches".

The enclosed report provides a summary of the data forthcoming from the monitoring, based on the latest information from all installations using the novel technology received in accordance with paragraph 3 along with the information required by Article 13(5) of the Regulation.

a) Brief description of the novel technology

The Flake Injection process has the capability to combine depolymerised recycled Polyethylene Terephthalate (rPET) with virgin material at different stages of a conventional PET production process for subsequent food contact use. The input material of the Flake Injection process is previously processed PET as detailed in Table 2 of ANNEX I of COMMISSION REGULATION (EU) 2022/1616 and is deliberately depolymerized (preprocessed) before it enters the high surface area decontamination polymerisation reactor. Referring to the flow scheme Appendix I: Flake Injection – PET Production Process; previously processed PET may be introduced directly to injection point 1. or partially depolymerised with ethylene glycol, in either a stir-tank reactor or an extruder, to a defined degree of polymerisation to correspond with that of the polymer in the PET production process at the injection points labelled 2 to 6 in the flow scheme or any points in-between. This initial depolymerisation process of the previously processed PET allows for filtration of the intermediate polymer to remove solid contaminants before the introduction of the recycled material into a PET production process at a blend rate of up to 100% recycled content. The high surface area decontamination polymerisation technology increases the Intrinsic Viscosity (IV) of the PET polymer and removes polymerisation by-products under high vacuum of less than 20mbar, with a high temperature greater than 260°C and with a residence time greater than 30 minutes. This high surface area polymerisation technology also serves as a Decontamination Technology to efficiently remove vapourised contaminants that may have been introduced into the process further upstream by the addition of previously processed PET. Following the high surface area polymerisation and decontamination, the polymer melt is filtered for either direct use, or granulation, in the manufacture of food contact materials or articles or for introduction into a Solid State Polycondensation (SSP) process or a Conditioning Silo should further processing be needed to meet the material parameters required for its end use.

b) Summary of the reasoning on the capability of the novel technology and the recycling process(es) to manufacture recycled plastic materials and articles that meet the requirements of Article 3 of Regulation (EC) No 1935/2004 and that are microbiologically safe.

Flake To Resin (FTR)

Ref. ANNEX II Table 1 (1) <u>Decontamination efficiency of a new post-consumer poly(ethylene terephthalate) (PET) recycling concept</u>. FRANK WELLE. Fraunhofer Institute for Process Engineering and Packaging (IVV), Giggenhauser Straße 35, 85354 Freising, Germany.

Table VI. Concentrations (determined using the HFIP extraction method) of the surrogates in the investigated PET samples of Trial 2 (cocktail A at 10 ml min⁻¹, 50% PCR flakes).

			Con	centration (ppm)			
	Toluene	Chloroform	Chlorobenzene	Phenyl cyclohexane	Methyl salicylate	Benzophenone	Lindane
Calculated contamination concentration	3295	5194	1255	327	1004	885	775
Before deep-cleansing	1999 ± 28	3075 ± 47	655 ± 9	163 ± 2	<1.0	345 ± 1	133 ± 1
After deep-cleansing (final product)	<2.7	<0.8	<0.9	<0.2	<1.0	<0.2	<0.8

The cleaning efficiencies for the applied surrogates are above or far above 99.9%. The high cleaning efficiencies are due to the high diffusion rates of compounds in the molten PET.

Based on EFSA's criteria for safety evaluation of PET recycling processes - if a recycling process is able to reduce an input reference contamination of 3 mg/kg PET to a Cres (Residual Concentration) not higher than a Cmod (Modelled Concentration) corresponding to the relevant migration criterion, the potential dietary exposure cannot be higher than $0.0025\,\mu\text{g/kg}$ bw/day and recycled PET manufactured with such recycling process is not considered of safety concern.

Ref. ANNEX II Table 1 (2) Fraunhofer Dossier-FTR 20061109.pdf

Reversed Approach

Based on Safety Evaluation of Polyethylene Terephthalate Chemical Re-cycling Processes. Frank Welle. 'Reversed Approach'.

Ref. ANNEX II Table 1 (3) <u>!chemical_recycling_submitted.pdf</u>

FTR: Calculated maximum concentration (Reference Contamination – the level of contamination that the process can remove, i.e. Cmod:Cres =1) corresponding to a migration of 0.1 μ g/l after storage for 365 d at 25 °C (EU cube, AP = 3.1, tau 1577 K, bottle wall thickness 200 μ m, density of PET 1.4 g/cm³). Decontamination Efficiency of 99.9%.

mm Hg (25°C)	°C	g.mol ⁻¹	FTR	Reference Contamination	Decontamination Efficiency	Cres	Cmod	
Vapour Pressure	BP	Mw	Surrogate	mg/kg	%	mg/kg	mg/kg	Cmod:Cres
28.4	110.6	92.1	Toluene	90	99.9%	0.09	0.09	1.0
197	61.1	119.4	Chloroform	100	99.9%	0.10	0.10	1.0
12	131.7	112.6	Chlorobenzene	90	99.9%	0.09	0.09	1.0
0.0343	222.9	152.2	Methyl Salicylate	130	99.9%	0.13	0.13	1.0
0.04	240.1	160.3	Phenyl Cyclohexane	140	99.9%	0.14	0.14	1.0
0.00193	305.4	182.2	Benzophenone	160	99.9%	0.16	0.16	1.0
9.40E-06	311.0	290.8	Lindane	310	99.9%	0.31	0.31	1.0

Artenius.

EFSA-Q-2011-00969 - EFSA refused to evaluate as out of the scope of Regulation (EC) 282/2008.

Ref. ANNEX II Table 1 (7) EFSA Letter Related to Artenius Unique Process.pdf

Ref. ANNEX II Table 1 (8) <u>Fraunhofer Institute. Challenge Test.pdf</u>

US FDA Guidance

Use of Recycled Plastics in Food Packaging (Chemistry Considerations): Guidance for Industry.

U.S. Department of Health and Human Services Food and Drug Administration Center for Food Safety and Applied Nutrition July 2021

VIII. Elimination of Data Recommendations for 3° Recycling Processes for PET and PEN

Based on a comprehensive review of all surrogate testing data submitted over the past decade for 3° recycling processes for PET and polyethylene naphthalate (PEN), FDA concludes that 3° recycling of PET or PEN by methanolysis or glycolysis results in the production of monomers or oligomers that are readily purified to produce a finished polymer that is suitable for food-contact use. Both 3° processes will clean the polyester sufficiently to allow it to be considered of suitable purity, even assuming 100% migration of residual surrogate to food. This is a significant difference from the surrogate testing of 2° recycling processes. Secondary recycling processes often produce PET that is insufficiently cleaned to withstand 100% migration calculations for the residual surrogates. Under these circumstances, FDA recommends additional migration tests to demonstrate that the finished PET meets the $1.5 \,\mu g/person/day$ EDI limit.

Based on a determination that 3° recycling processes produce PET or PEN of suitable purity for foodcontact use, FDA no longer recommends that such recyclers submit data for agency evaluation. Because 3° processes for polymers other than PET and PEN were not the subject of FDA reviews, recyclers who wish to engage in 3° recycling of polymers other than PET and PEN are encouraged to submit data for evaluation.

Ref. ANNEX II Table 1 (9) Recycled-Plastics-Food-Packaging-Chemistry-ConsiderationsGuidance-04112022-1321.pdf

c) List a list of all substances with a molecular weight below 1000 Dalton found in the plastic inputs and recycled plastic output

As developer of the Novel Technology, PET-Europe has coordinated with the recyclers regarding the selection of the sampling strategy, the analysis to be performed and the selection of a third-party laboratory. The choice of the laboratory was based on its experience and expertise in analysing PET samples, the relevance of its analytical equipment and validated methods as well as the capability to identify and to risk assess non-intentionally added substances (NIAS) taking into account the particularity of this specific technology.

The results of the Targeted analysis of inorganic substances by ICP-MS are not included due to an issue with metal contamination of samples during the milling phase used for sample preparation rendering the ICP-MS results unreliable, The laboratory is in the process of rectifying and repeating the analysis but with the large amount of samples to test this will inevitably be delayed. Therefore, the outcome of the analysis will be added to the report as soon as they become available.

Volatiles

Pormula CAS	Oit						Classina
Dipropylene glycol		Name	Formula	CAS			Cleaning efficiency, %
1-Propanol. 2, 2'oxybib-	1	1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3	106-62-7	8565.71	2170.85	74.7
Table Care		Dipropylene glycol	C6H14O3	110-98-5	8315.69	2958.10	64.4
Undecane, 2,3dimethyl-	1	1-Propanol, 2,2'oxybis-	C6H14O3	108-61-2	7452.90	2525.77	66.1
1-Dodecanol C12H260 112:53-8 524.63	E	Ethanol, 2-(dodecyloxy)-	C14H30O2	4536-30-5	4499.72		100.0
Octanoic acid C8H16O2 124-07-2 421.32	ι	Jndecane, 2,3dimethyl-	C13H28	17312-77-5	628.75		100.0
1-Heptanol, 2-propyl-	1	1-Dodecanol	C12H26O	112-53-8	524.63		100.0
Deciration	C	Octanoic acid	C8H16O2	124-07-2	421.32		100.0
Deciration	ដ [1	1-Heptanol, 2-propyl-	C10H22O	10042-59-8	303.55		100.0
Decimane	₹Ŀ	1-Eicosanol	C20H42O	629-96-9	230.29		100.0
7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione C17H24O3 82304-66-3 51.68 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 23.35 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 14.86 102.06 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 23.35 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 24.86 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 23.85 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 24.86 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 24.86 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 23.85 2.5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 24.86 2.5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 24.86 2.5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 24.86 2.5-di-tert-Butyl-1,4-benzoquinone C14H20 2460-77-7 25.55 6.14 2.5-di-tert-Butyl-1,4-benzoquinone C14H20 2460-77-7 27.88 2.5-di-tert-Butyl-1,4-benzoquinone	S	Decanal	C10H20O	112-31-2	177.07		100.0
2,5-di-tert-Butyl-1,4benzoquinone	[D-Limonene	C10H16	5989-27-5	144.01		100.0
2,5-di-tert-Butyl-1,4benzoquinone C14H20O2 2460-77-7 21.40 2,5-di-tert-Butyl-1,4benzoquinone C14H20O2 2460-77-7 14.86 102.06 Nonanal C9H18O 124-19-6 102.06 Nonanal C9H18O 124-19-6 102.06 Nonanal C4H18O 124-19-6 102.06 Nonanal C4H18O 124-19-6 102.06 Nonanal C4H18O 112-54-9 605.10 87.58 1-Hexanol, 2-ethyl- C4H18O 104-76-7 305.85 Nonanal C4H18O 124-19-6 285.43 0-Terpineol C14H18O 98-55-5 79.40 Toluene C7H18O 108-88-3 17.42 m-Xylene (Benzene, 1,3-dimethyl) C4H18O 108-88-3 17.42 m-Xylene (Benzene, 1,3-5-trimethyl) C4H18O 108-88-3 12.93 C4H18O C4H1	7	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	C17H24O3	82304-66-3	51.68		100.0
Name		2,5-di-tert-Butyl-1,4benzoquinone	C14H20O2	2460-77-7	23.35		100.0
Nonanal C9H18O 124-19-6 102.06		2,5-di-tert-Butyl-1,4benzoquinone	C14H20O2	2460-77-7	21.40		100.0
Name Formula CAS Input Dutputing Input I		2,5-di-tert-Butyl-1,4benzoquinone	C14H20O2	2460-77-7	14.86		100.0
Ethanol, 2-(dodecyloxy)-	1	Nonanal	C9H18O	124-19-6		102.06	
Ethanol, 2-(dodecyloxy)-							
Ethanol, 2-{dodecyloxy}- C ₁₄ H ₃₀ O ₂ 4536-30-5 1368.96 Dodecanal C ₁₃ H ₂₄ O 112-54-9 605.10 87.58 1-Hexanol, 2-ethyl- CaHisO 104-76-7 305.85 Nonanal CaHisO 124-19-6 285.43 α-Terpineol C ₁₆ H ₁₈ O 98-55-5 79.40 Toluene ChH 108-88-3 17.42 m-Xylene (Benzene, 1,3-dimethyl) CaHis 108-88-3 17.42 Chloroxylenol C ₃ H ₃ ClO 88-04-0 10.84 Mesitylene (Benzene, 1,3-5-trimethy) ChH ₁₂ 108-67-8 10.24 Ethylbenzene CaHis 100-41-4 8.46 Ethylbenzene CaHis 100-41-4 8.46 Enzene, 1-ethyl-3methyl- CaHis 106-42-3 5.74 Benzene, 1-ethyl-3methyl- CaHis 620-14-4 3.89 Benzene, 1-ethyl-4methyl- CaHis 629-59-4 44.69 1-Judecanol CiHis-4 112-42-5 238.63 Tetradecane CaHis 629-59-4 46.90 Name Formula CAS Input Unput Unput					Input	Outnutue	Cleaning
Ethanol, 2-(dodecyloxy)-		Name	Formula	CAS			efficiency,
Dodecanal	-					,	%
1-Hexanol, 2-ethyl-							100.0
Nonanal C-HisO 124-19-6 285.43 C-Terpineol Collisio 98-55-5 79.40 Tollene C-His 108-88-3 17.42 C-His 108-87-8 10.24 C-His 108-67-8 10.24 C-His 10.	- 1		C ₁₂ H ₂₄ O	112-54-9	605.10	87.58	-
C10H1sO 98-55-5 79.40	1	I-Hexanol, 2-ethyl-	C8H18O	104-76-7	305.85		100.0
Toluene	1	Nonanal	C9H18O	124-19-6	285.43		100.0
M-Xylene (Benzene, 1,3-dimethyl)	0	x-Terpineol	C10H18O	98-55-5	79.40		100.0
Chloroxylenol C ₈ H ₉ CIO 88-04-0 10.84 Mesitylene (Benzene, 1,3,5-trimethy) C ₉ H ₁₂ 108-67-8 10.24 Ethylbenzene	1	l'oluene l'acceptant de la company de la com	C7H8	108-88-3	17.42		100.0
Mesitylene (Benzene, 1,3,5-trimethy) C3H12 108-67-8 10.24 Ethylbenzene CaH10 100-41-4 8.46 P-Xylene (Benzene, 1,4-dimethyl-) C3H10 106-42-3 5.74 Ethylbenzene CaH10 106-42-3 5.74 Ethylbenzene CaH10 106-42-3 5.74 Ethylbenzene CaH10 106-42-3 5.74 Enzene, 1-ethyl-Zmethyl- C9H12 611-14-3 4.35 620-14-4 3.89 Enzene, 1-ethyl-3methyl- C9H12 620-14-4 3.89 Enzene, 1-ethyl-4methyl- C9H12 622-96-8 3.85 1,3-Dioxolane, 2-methyl- C4HxO2 497-26-7 1997.90 C4Tanoic acid, ethyl ester C10Hx0O2 106-32-1 44.69 1-Undecanol C11Hx4O 112-42-5 238.63 Tetradecane C14Hx0 629-59-4 46.90 C4Hx0O C4HxO2 C4HxO3 C4HxO	r	n-Xylene (Benzene, 1,3-dimethyl)	C8H10	108-38-3	12.93		100.0
P.Xylene (Benzene, 1,4-dimethyl-) CaH10 106-42-3 5.74 Benzene, 1-ethyl-2methyl- CoH12 611-14-3 4.35 Benzene, 1-ethyl-3methyl- CoH12 622-96-8 3.85 1,3-Dioxolane, 2-methyl- CaH8O2 497-26-7 1997.90 Octanoic acid, ethyl ester C10H20O2 106-32-1 44.69 1-Undecanol C11H24O 112-42-5 238.63 Tetradecane C14H30 629-59-4 46.90 Name Formula CAS Input μg/kg PET //kg PET Acetic acid, methoxy- CaH6O3 625-45-6 99547.49 Dipropylene glycol CaH14O3 110-98-5 10661.55 1-Propanol, 2-(2-hydroxypropoxy)- CaH14O3 110-98-5 9587.44 Ethanol, 2-(dodecyloxy)- CaH300 110-98-5 9587.44 Ethanol, 2-(dodecyloxy)- CaH300 124-19-6 801.21 Phthalic acid, diisobutyl ester C16H2O4 84-69-5 225.12 2-Decenal, (E)- C16H30 313-81-3 168.56 1-Octadecanol C18H30 112-92-5 146.82 Dodecanal C10H20O 112-31-2 129.62 Dodecanal C12H24O 112-54-9 77.10 Tetradecane C14H30 C2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 25.55 6.14 2,5	7	Chloroxylenol	C ₈ H ₉ ClO	88-04-0	10.84		100.0
P.Xylene (Benzene, 1,4-dimethyl-) CaH10 106-42-3 5.74 Benzene, 1-ethyl-2methyl- CoH12 611-14-3 4.35 Benzene, 1-ethyl-3methyl- CoH12 622-96-8 3.85 1,3-Dioxolane, 2-methyl- CaH8O2 497-26-7 1997.90 Octanoic acid, ethyl ester C10H20O2 106-32-1 44.69 1-Undecanol C11H24O 112-42-5 238.63 Tetradecane C14H30 629-59-4 46.90 Name Formula CAS Input μg/kg PET /kg PET Acetic acid, methoxy- C146O3 625-45-6 99547.49 Dipropylene glycol C4H4O3 110-98-5 10661.55 1-Propanol, 2-{2-hydroxypropoxy}- C4H4O3 110-98-5 9587.44 Ethanol, 2-{dodecyloxy}- C14H30 110-98-5 9587.44 Ethanol, 2-{dodecyloxy}- C14H30 124-19-6 801.21 Phthalic acid, diisobutyl ester C16H2O4 84-69-5 225.12 2-Decenal, (E}- C10H18O 3913-81-3 168.56 1-Octadecanol C18H30 112-92-5 146.82 Dodecanal C10H26O 112-31-2 129.62 Dodecanal C10H26O 112-31-2 129.62 Dodecanal C12H24O 112-54-9 77.10 Tetradecane C14H30O2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone C14H26O2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone C14H26O2 2460-77-7 25.55 6.14 D-Xylene C4H10 106-42-3 5.77	2 7	Mesitylene (Benzene, 1,3,5-trimethy)	C9H12	108-67-8	10.24		100.0
P.Xylene (Benzene, 1,4-dimethyl-) CaH10 106-42-3 5.74 Benzene, 1-ethyl-2methyl- CoH12 611-14-3 4.35 Benzene, 1-ethyl-3methyl- CoH12 622-96-8 3.85 1,3-Dioxolane, 2-methyl- CaH8O2 497-26-7 1997.90 Octanoic acid, ethyl ester C10H20O2 106-32-1 44.69 1-Undecanol C11H24O 112-42-5 238.63 Tetradecane C14H30 629-59-4 46.90 Name Formula CAS Input μg/kg PET /kg PET Acetic acid, methoxy- C146O3 625-45-6 99547.49 Dipropylene glycol C4H4O3 110-98-5 10661.55 1-Propanol, 2-{2-hydroxypropoxy}- C4H4O3 110-98-5 9587.44 Ethanol, 2-{dodecyloxy}- C14H30 110-98-5 9587.44 Ethanol, 2-{dodecyloxy}- C14H30 124-19-6 801.21 Phthalic acid, diisobutyl ester C16H2O4 84-69-5 225.12 2-Decenal, (E}- C10H18O 3913-81-3 168.56 1-Octadecanol C18H30 112-92-5 146.82 Dodecanal C10H26O 112-31-2 129.62 Dodecanal C10H26O 112-31-2 129.62 Dodecanal C12H24O 112-54-9 77.10 Tetradecane C14H30O2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone C14H26O2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone C14H26O2 2460-77-7 25.55 6.14 D-Xylene C4H10 106-42-3 5.77	₽ E	Ethylbenzene	C8H10	100-41-4	8.46		100.0
Benzene, 1-ethyl-3methyl-		o-Xylene (Benzene, 1,4-dimethyl-)	C8H10	106-42-3	5.74		100.0
Benzene, 1-ethyl-4methyl-	E	Benzene, 1-ethyl-2methyl-	C9H12	611-14-3	4.35		100.0
1,3-Dioxolane, 2-methyl-Octanoic acid, ethyl ester	E	Benzene, 1-ethyl-3methyl-	C9H12	620-14-4	3.89		100.0
Octanoic acid, ethyl ester	E	Benzene, 1-ethyl-4methyl-	C9H12	622-96-8	3.85		100.0
T-Undecanol C11H24O 112-42-5 238.63 Tetradecane C14H30 629-59-4 46.90 Name Formula CAS Input μg/kg PET / kg PET Acetic acid, methoxy- C3H6O3 625-45-6 99547.49 Dipropylene glycol C4H14O3 110-98-5 10661.55 1-Propanol, 2-{2-hydroxypropoxy}- C4H14O3 110-98-5 9984.90 Dipropylene glycol C4H14O3 110-98-5 9984.90 Dipropylene glycol C4H14O3 110-98-5 9587.44 Ethanol, 2-{dodecyloxy}- C14H30O2 4536-30-5 3735.35 47.00 Nonanal C0H18O 124-19-6 801.21 Phthalic acid, diisobutyl ester C16H22O4 84-69-5 225.12 2-Decenal, (E)- C10H18O 3913-81-3 168.56 1-Octadecanol C18H3SO 112-92-5 146.82 Dodecanal C10H26O 112-31-2 129.62 Dodecanal C12H24O 112-54-9 77.10 Tetradecane C14H30 629-59-4 51.20 87.84 Nonanoic acid C9H18O 112-05-0 38.81 2,5-di-tert-Butyl-1,4-benzoquinone C14H26O2 2460-77-7 27.88 2,5-di-tert-Butyl-1,4-benzoquinone C14H26O2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone C14H26O2 2460-77-7 15.41 p-Xylene C4H10 106-42-3 5.77	1	1,3-Dioxolane, 2-methyl-	C4H8O2	497-26-7		1997.90	
Name Formula CAS Input Dutputug /kg PET /kg PET	(Octanoic acid, ethyl ester	C10H20O2	106-32-1		44.69	-
Name Formula CAS Input	1	1-Undecanol	C11H24O	112-42-5		238.63	-
Name Formula CAS Input Uutputtg /kg PET (4 / kg PET 4 / kg PET (4 / kg PET 4 / kg PET 4 / kg PET (4 / kg PET 4 / kg PET 4 / kg PET (4 / kg PET 4 / kg PET (4 / kg PET 4 / kg PET 4 / kg PET 4 / kg PET (4 / kg PET 4 / kg PE	7	Tetradecane	C14H30	629-59-4		46.90	-
Name Formula CAS Input Uutputtg /kg PET (4 / kg PET 4 / kg PET (4 / kg PET 4 / kg PET 4 / kg PET (4 / kg PET 4 / kg PET 4 / kg PET (4 / kg PET 4 / kg PET (4 / kg PET 4 / kg PET 4 / kg PET 4 / kg PET (4 / kg PET 4 / kg PE							
Dipropylene glycol		Name	Formula	CAS			Cleaning efficiency, %
1-Propanol, 2-(2-hydroxypropoxy)- CaH14O3 106-62-7 9984.90	1	Acetic acid, methoxy-	C3H6O3	625-45-6	99547.49		100.0
Dipropylene glycol C6H14O3 110-98-5 9587.44 Ethanol, 2-{dodecyloxy}- C14H30O2 4536-30-5 3735.35 47.00 Nonanal C0H18O 124-19-6 801.21 Phthalic acid, diisobutyl ester C16H22O4 84-69-5 225.12 2-Decenal, (E)- C10H18O 3913-81-3 168.56 1-Octadecanol C18H38O 112-92-5 146.82 Decanal C10H20O 112-31-2 129.62 Dodecanal C12H24O 112-54-9 77.10 Tetradecane C14H30 629-59-4 51.20 87.84 Nonanoic acid C0H18O2 112-05-0 38.81 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 27.88 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 15.41 p-Xylene C8H10 106-42-3 5.77		Dipropylene glycol	C ₆ H ₁₄ O ₃	110-98-5	10661.55		100.0
Ethanol, 2-(dodecyloxy)- C14H30O2 4536-30-5 3735.35 47.00	1	1-Propanol, 2-(2-hydroxypropoxy)-	C ₆ H ₁₄ O ₃	106-62-7	9984.90		100.0
Nonanal CoH18O 124-19-6 801.21	[Dipropylene glycol	C6H14O3	110-98-5	9587.44		100.0
Phthalic acid, diisobutyl ester 2-Decenal, (E)- 1-Octadecanol Decanal ClaH20 Dodecanal ClaH20 Tetradecane ClaH30 ClaH30 ClaH30 ClaH240 ClaH240 ClaH240 ClaH240 ClaH30 ClaH240 ClaH30 Cl	E	Ethanol, 2-(dodecyloxy)-	C14H30O2	4536-30-5	3735.35	47.00	98.7
2-Decenal, (E)- 1-Octadecanol C18H38O 112-92-5 146.82 Decanal C10H29O 112-31-2 129.62 Dodecanal C12H24O 112-54-9 77.10 Tetradecane C14H30 C29-59-4 51.20 87.84 Nonanoic acid C3H38O 2,5-di-tert-Butyl-1,4-benzoquinone C14H29O2 2,5-di-tert-Butyl-1,4-benzoquinone	1	Nonanal	C9H18O	124-19-6	801.21		100.0
1-Octadecanol	F	Phthalic acid, diisobutyl ester	C16H22O4	84-69-5	225.12		100.0
Tetradecane Cl4H30 629-59-4 51.20 87.84 Nonanoic acid CgH18O2 112-05-0 38.81 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 27.88 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 15.41 p-Xylene CgH1g 106-42-3 5.77	2	2-Decenal, (E)-	C10H18O	3913-81-3	168.56		100.0
Tetradecane Cl4H30 629-59-4 51.20 87.84 Nonanoic acid CgH18O2 112-05-0 38.81 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 27.88 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 15.41 p-Xylene CgH1g 106-42-3 5.77	<u>"</u>	1-Octadecanol	C18H38O	112-92-5	146.82		100.0
Tetradecane Cl4H30 629-59-4 51.20 87.84 Nonanoic acid CgH18O2 112-05-0 38.81 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 27.88 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 15.41 p-Xylene CgH1g 106-42-3 5.77	<u> </u>	Decanal	C10H20O		129.62		100.0
Tetradecane Cl4H30 629-59-4 51.20 87.84 Nonanoic acid CgH18O2 112-05-0 38.81 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 27.88 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone Cl4H2gO2 2460-77-7 15.41 p-Xylene CgH1g 106-42-3 5.77	SA	Oodecanal		 			100.0
Nonanoic acid C ₉ H ₁₈ O ₂ 112-05-0 38.81 2,5-di-tert-Butyl-1,4-benzoquinone C ₁₄ H ₂₀ O ₂ 2460-77-7 27.88 2,5-di-tert-Butyl-1,4-benzoquinone C ₁₄ H ₂₀ O ₂ 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone C ₁₄ H ₂₀ O ₂ 2460-77-7 15.41 p-Xylene C ₈ H ₁₀ 106-42-3 5.77						87.84	-71.6
2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 27.88 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 15.41 p-Xylene C8H10 106-42-3 5.77	-				38.81		100.0
2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 25.55 6.14 2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 15.41 p-Xylene C8H10 106-42-3 5.77	-						100.0
2,5-di-tert-Butyl-1,4-benzoquinone C14H20O2 2460-77-7 15.41 p-Xylene C8H10 106-42-3 5.77						6.14	76.0
p-Xylene C ₄ H ₁₀ 106-42-3 5.77				 			100.0
							100.0
					27	2423.53	
Dipropylene glycol C ₆ H ₁₄ O ₃ 110-98-5 1528.43							-
Dipropylene glycol C ₆ H ₁₄ O ₃ 110-98-5 2166.73				 			
7,9-Di-tert-butyl-oxaspiro(4,5)deca6,9-diene-2,8-dione C ₁₇ H ₂₄ O ₃ 82304-66-3 25.03							-
n-Hexadecanoic acid C ₁₆ H ₃₂ O ₂ 57-10-3 <10							-

Volatiles (contd)

-	T					
				Input	Outputµg	Cleaning
	Name	Formula	CAS	µg/kg PET	/kg PET	efficiency,
				μg/ kg FE1	/ NB FEI	%
	p-Cymene	C10H14	99-87-6	5860.05		100.0
	6-Methyl-1-octanol	C9H2OO	110453-78-6	4008.33		100.0
	Dipropylene glycol	C6H14O3	110-98-5	3296.64		100.0
	Phthalic acid, butyl tetradecyl ester	C26H42O4	-	202.28		100.0
	Dipropylene glycol	C6H14O3	110-98-5	181.62		100.0
	Phthalic acid, butyl tetradecyl ester	C26H42O4	110-30-3	114.34		100.0
	1-Undecanol		112-42-5	79.20	53.40	32.6
		C11H24O	2460-77-7	64.81	64.81	0.0
4	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2			04.81	
SAMPLE 4	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	C17H24O3	82304-66-3	53.50		100.0
Ž	1,4-benzoquinone	C14H20O2	2460-77-7	53.50		100.0
S	D-Limonene	C10H16	5989-27-5	32.07		100.0
	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	C17H24O3	82304-66-3	14.46	4.82	66.7
	Dodecanal	C12H24O	112-54-9	9.33		100.0
	1-Hexadecanol, 2-methyl-	C 17H36O	2490-48-4	3.84		100.0
	Dipropylene glycol	C6H14O3	110-98-5		1732.47	-
	Dipropylene glycol	C6H14O3	110-98-5		1199.75	-
	Dipropylene glycol	C6H14O3	110-98-5		1703.76	-
	p-Benzoquinone, 2,6-di-tert-butyl-	C 14H20O2	719-22-2		69.11	-
	Dipropylene glycol	C6H14O3	110-98-5		5.43	-
						Cleaning
	N	F1-	646	Input	Outputµg	_
	Name	Formula	CAS	μg/kg PET	/kg PET	efficiency,
						%
	Ethanol, 2-(dodecyloxy)	C14H30O2	4536-30-5	53.68	63.86	-19.0
	Dodecanal	C12H24O	112-54-9	53.60		100.0
	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	11.11	13.26	-19.4
Ä.	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	9.76	9.82	-0.6
SAMPLE 5	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	C17H24O3	82304-66-3	4.00		100.0
SA	Diisobutyl phthalate	C16H22O4	84-69-5	1.63	1.92	-17.8
	2-Propanol, 1,1'oxybis-	C6H14O3	110-98-5		8833.31	-
i						
	Dipropylene glycol	C6H14O3	110-98-5		5489.31	-
		C6H14O3	110-98-5 110-98-5		5489.31 6351.70	-
	Dipropylene glycol					-
	Dipropylene glycol					
	Dipropylene glycol Dipropylene glycol	C6H14O3	110-98-5	Input		Cleaning
	Dipropylene glycol			Input μg/kg PET	6351.70	Cleaning efficiency,
	Dipropylene glycol Dipropylene glycol Name	C ₆ H ₁₄ O ₃ Formula	110-98-5 CAS	μg/kg PET	6351.70 Outputµg /kg PET	Cleaning efficiency, %
	Dipropylene glycol Dipropylene glycol Name	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O	110-98-5 CAS	μg/kg PET 2924.22	6351.70 Outputμg	Cleaning efficiency, % 60.8
	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O	110-98-5 CAS 124-19-6 112-31-2	μg/kg PET 2924.22 1541.90	6351.70 Outputμg /kg PET 1145.84	Cleaning efficiency, % 60.8 100.0
	Dipropylene glycol Dipropylene glycol Name	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O	110-98-5 CAS	μg/kg PET 2924.22	6351.70 Outputμg /kg PET 1145.84	Cleaning efficiency, % 60.8 100.0
E 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O	110-98-5 CAS 124-19-6 112-31-2	μg/kg PET 2924.22 1541.90	6351.70 Outputµg /kg PET 1145.84	Cleaning efficiency, % 60.8 100.0
MPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O ₂	110-98-5 CAS 124-19-6 112-31-2 112-05-0	μg/kg PET 2924.22 1541.90 483.84	6351.70 Outputµg /kg PET 1145.84	Cleaning efficiency, % 60.8 100.0
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-(1-methylethenyl)-	$\begin{array}{c} C_6H_{14}O_3 \\ \\ Formula \\ \\ C_9H_{13}O \\ \\ C_{10}H_{20}O \\ \\ C_9H_{13}O_2 \\ \\ C_{10}H_{18}O \\ \\ C_{2}H_{4}O_2 \\ \end{array}$	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2	μg/kg PET 2924.22 1541.90 483.84 348.10	6351.70 Outputµg /kg PET 1145.84	Cleaning efficiency, % 60.8 100.0 100.0 100.0 100.0
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-(1-methylethenyl)- Acetic acid p-Xylene	$\begin{array}{c} C_6H_{14}O_3 \\ \\ Formula \\ \\ C_9H_{18}O \\ \\ C_{10}H_{20}O \\ \\ C_9H_{18}O_2 \\ \\ C_{10}H_{18}O \\ \\ C_{2}H_{4}O_2 \\ \\ C_{6}H_{10} \\ \end{array}$	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16	Outputµg /kg PET 1145.84	Cleaning efficiency, % 60.8 100.0 100.0 100.0 100.0 100.0
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-(1-methylethenyl)- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl-		110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80	Outputµg /kg PET 1145.84	Cleaning efficiency, % 60.8 100.0 10
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-(1-methylethenyl)- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene		110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16	Outputµg /kg PET 1145.84	Cleaning efficiency, % 60.8 100.0 100.0 100.0 100.0 100.0 100.0
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-(1-methylethenyl)- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl-		110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80	Outputµg /kg PET 1145.84	Cleaning efficiency, % 60.8 100.0 10
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-(1-methylethenyl)- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene		110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80	Outputµg /kg PET 1145.84	Cleaning efficiency, % 60.8 100.0 10
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O ₂ C ₁₀ H ₁₈ O C ₂ H ₄ O ₂ C ₆ H ₁₀ C ₉ H ₁₂ C ₇ H ₈ C ₄ H ₆ O	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63	Outputµg /kg PET 1145.84 5155.20	Cleaning efficiency, % 60.8 100.0 100.0 100.0 100.0 100.0 100.0 100.0 Cleaning
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-(1-methylethenyl)- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene		110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63	Outputµg /kg PET 1145.84 5155.20	Cleaning efficiency, % 60.8 100.0 100.0 100.0 100.0 100.0 100.0 Cleaning efficiency,
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O ₂ C ₁₀ H ₁₈ O C ₂ H ₄ O ₂ C ₆ H ₁₀ C ₉ H ₁₂ C ₇ H ₈ C ₄ H ₆ O	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63	Outputµg /kg PET 1145.84 5155.20	Cleaning efficiency, % 60.8 100.0 100.0 100.0 100.0 100.0 100.0 100.0 Cleaning
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O ₂ C ₁₀ H ₁₈ O C ₂ H ₄ O ₂ C ₆ H ₁₀ C ₉ H ₁₂ C ₇ H ₈ C ₄ H ₆ O	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63	Outputµg /kg PET 1145.84 5155.20	Cleaning efficiency, % 60.8 100.0 100.0 100.0 100.0 100.0 100.0 Cleaning efficiency,
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name	$ \begin{aligned} & \text{Formula} \\ & $	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET	Cleaning efficiency, % 60.8 100.0 10
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name	$ \begin{aligned} & \text{Formula} \\ & $	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS 2517-43-3	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET 4499.63	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET 0.00	Cleaning efficiency, % 60.8 100.0 10
SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name 1-Butanol, 3-methoxy Ethanol, 2-(dodecyloxy)	$ \begin{aligned} & $	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS 2517-43-3 4536-30-5	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET 4499.63 964.38	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET 0.00 0.00	Cleaning efficiency, % 60.8 100.0 10
	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name 1-Butanol, 3-methoxy Ethanol, 2-(dodecyloxy) Dodecanal	$ \begin{aligned} & $	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS 2517-43-3 4536-30-5 112-54-9	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET 4499.63 964.38 721.23	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET 0.00 0.00	Cleaning efficiency, % 60.8 100.0 10
	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name 1-Butanol, 3-methoxy Ethanol, 2-(dodecyloxy) Dodecanal Nonanal	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O C ₁₀ H ₁₈ O C ₂ H ₄ O ₂ C ₈ H ₁₀ C ₉ H ₁₂ C ₇ H ₈ C ₄ H ₆ O Formula C5H12O2 C14H3OO2 C12H24O C9H18O	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS 2517-43-3 4536-30-5 112-54-9 124-19-6	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET 4499.63 964.38 721.23 434.37	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET 0.00 0.00	Cleaning efficiency, % 60.8 100.0 10
	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name 1-Butanol, 3-methoxy Ethanol, 2-(dodecyloxy) Dodecanal Nonanal Undecanal D-Limonene	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O C ₁₀ H ₁₈ O C ₂ H ₄ O ₂ C ₈ H ₁₀ C ₉ H ₁₂ C ₇ H ₈ C ₄ H ₆ O Formula C5H12O2 C14H3OO2 C14H3OO2 C12H24O C9H18O C11H22O C10H16	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS 2517-43-3 4536-30-5 112-54-9 124-19-6 112-44-7 5989-27-5	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET 4499.63 964.38 721.23 434.37 110.88	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET 0.00 0.00 101.51	Cleaning efficiency, % 60.8 100.0 10
SAMPLE 7 SAMPLE 6	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name 1-Butanol, 3-methoxy Ethanol, 2-(dodecyloxy) Dodecanal Nonanal Undecanal D-Limonene Dipropylene glycol	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O C ₁₀ H ₁₈ O C ₂ H ₄ O ₂ C ₈ H ₁₀ C ₉ H ₁₂ C ₇ H ₈ C ₄ H ₆ O Formula C5H12O2 C14H30O2 C12H24O C9H18O C11H22O C10H16 C6H14O3	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS 2517-43-3 4536-30-5 112-54-9 124-19-6 112-44-7 5989-27-5 110-98-5	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET 4499.63 964.38 721.23 434.37 110.88	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET 0.00 0.00 101.51	Cleaning efficiency, % 60.8 100.0 10
	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-(1-methylethenyl)- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name 1-Butanol, 3-methoxy Ethanol, 2-(dodecyloxy) Dodecanal Nonanal Undecanal D-Limonene Dipropylene glycol Dipropylene glycol	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O C ₁₀ H ₁₈ O C ₂ H ₄ O ₂ C ₈ H ₁₀ C ₉ H ₁₂ C ₇ H ₈ C ₄ H ₆ O Formula C5H12O2 C14H30O2 C12H24O C9H18O C11H22O C10H16 C6H14O3 C6H14O3	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS 2517-43-3 4536-30-5 112-54-9 124-19-6 112-44-7 5989-27-5 110-98-5 110-98-5	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET 4499.63 964.38 721.23 434.37 110.88	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET 0.00 0.00 101.51 770.38 291.53	Cleaning efficiency, % 60.8 100.0 10
	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name 1-Butanol, 3-methoxy Ethanol, 2-(dodecyloxy) Dodecanal Nonanal Undecanal D-Limonene Dipropylene glycol Dipropylene glycol Dipropylene glycol	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O C ₁₀ H ₁₈ O C ₂ H ₄ O ₂ C ₈ H ₁₀ C ₉ H ₁₂ C ₇ H ₈ C ₄ H ₆ O Formula C5H12O2 C14H30O2 C12H24O C9H18O C11H22O C10H16 C6H14O3 C6H14O3 C6H14O3	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS 2517-43-3 4536-30-5 112-54-9 124-19-6 112-44-7 5989-27-5 110-98-5 110-98-5	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET 4499.63 964.38 721.23 434.37 110.88	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET 0.00 0.00 101.51 770.38 291.53 366.56	Cleaning efficiency, % 60.8 100.0 10
	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name 1-Butanol, 3-methoxy Ethanol, 2-(dodecyloxy) Dodecanal Nonanal Undecanal D-Limonene Dipropylene glycol Dipropylene glycol Dipropylene glycol Linalool	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O C ₁₀ H ₁₈ O C ₂ H ₄ O ₂ C ₈ H ₁₀ C ₉ H ₁₂ C ₇ H ₈ C ₄ H ₆ O Formula C5H12O2 C14H30O2 C12H24O C9H18O C11H22O C10H16 C6H14O3 C6H14O3 C6H14O3 C10H18O	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS 2517-43-3 4536-30-5 112-54-9 124-19-6 112-44-7 5989-27-5 110-98-5 110-98-5 110-98-5 78-70-6	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET 4499.63 964.38 721.23 434.37 110.88	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET 0.00 0.00 101.51 770.38 291.53 366.56 20.72	Cleaning efficiency, % 60.8 100.0 10
	Dipropylene glycol Dipropylene glycol Name Nonanal Decanal Nonanoic acid Cyclohexanol, 2-methyl-5-{1-methylethenyl}- Acetic acid p-Xylene Benzene, 1,2,4-trimethyl- Toluene 2-Butenal Name 1-Butanol, 3-methoxy Ethanol, 2-(dodecyloxy) Dodecanal Nonanal Undecanal D-Limonene Dipropylene glycol Dipropylene glycol Dipropylene glycol	C ₆ H ₁₄ O ₃ Formula C ₉ H ₁₈ O C ₁₀ H ₂₀ O C ₉ H ₁₈ O C ₁₀ H ₁₈ O C ₂ H ₄ O ₂ C ₈ H ₁₀ C ₉ H ₁₂ C ₇ H ₈ C ₄ H ₆ O Formula C5H12O2 C14H30O2 C12H24O C9H18O C11H22O C10H16 C6H14O3 C6H14O3 C6H14O3	110-98-5 CAS 124-19-6 112-31-2 112-05-0 619-01-2 64-19-7 106-42-3 95-63-6 108-88-3 123-73-9 CAS 2517-43-3 4536-30-5 112-54-9 124-19-6 112-44-7 5989-27-5 110-98-5 110-98-5 110-98-5 78-70-6 98-55-5	μg/kg PET 2924.22 1541.90 483.84 348.10 129.14 61.16 35.80 21.63 Input μg/kg PET 4499.63 964.38 721.23 434.37 110.88	Outputµg /kg PET 1145.84 5155.20 Outputµg /kg PET 0.00 0.00 101.51 770.38 291.53 366.56	Cleaning efficiency, % 60.8 100.0 10

Volatiles (contd)

						Cleaning
	Name	Formula	CAS	Input	Outputµg	efficiency,
	Name	Formula	CA3	μg/kg PET	/kg PET	% %
	Dipropylene glycol	C6H14O3	110-98-5	7239.35	0.00	100.0
	Dipropylene glycol	C6H14O3	110-98-5	4267.60	0.00	100.0
	1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3	106-62-7	3991.76		100.0
	Nonanal	C9H18O	124-19-6	538.40	116.08	78.4
	1-Undecanol	C11H24O	112-42-5	126.28		100.0
	1-Hexadecanol, 2methyl-	C17H36O	2490-48-4	85.52		100.0
	D-Limonene	C10H16	5989-27-5	25.64		100.0
	L-α-Terpineol	C10H18O	10482-56-1	15.64		100.0
00	Diphenyl ether	C12H10O	101-84-8	3.96		100.0
E	Naphthalene, 2ethenyl-	C12H10	827-54-3	3.04		100.0
SAMPLE	Benzene	C6H6	71-43-2	1.89	0.00	100.0
SA	Benzyl alcohol	C ₇ H ₈ O	100-51-6		7.14	
	Decanal	C10H20O	112-31-2		78.40	
	Ethanol, phenoxy-	C8H10O2	122-99-6		24.60	
	Nonanoic acid	C9H18O2	112-05-0			-
	Biphenyl	C12H10	92-52-4		4.03	
	Diphenyl ether	C12H10O	101-84-8		8.13	
	2,4-Di-ertbutylphenol	C14H22O	96-76-4		13.32	
	Isopropyl myristate	C17H34O2	110-27-0		53.54	
	Benzenesulfonamide N-butyl-	C10H15NO2S	3622-84-2		<1	
						Cleaning
	Name	Formula	CAS	Input	Outputµg	efficiency,
				μg/kg PET	/kg PET	%
	Dodecanal	C12H24O	112-54-9	586.00	83.17	85.8
6	Nonanal	C9H18O	124-19-6	237.86	71.19	70.1
PE	1-Undecanol	C11H24O	112-42-5	129.59	129.59	0.0
SAMPLE	Mesitylene	C9H12	108-67-8	10.24		100.0
Š	Benzene, 1,3dimethyl-	C8H10	108-38-3	5.74		100.0
	Benzene, 1ethyl-3-methyl-	C9H12	620-14-4	3.89		100.0
					0.4	Cleaning
	Name	Formula	CAS	Input	Outputµg	efficiency,
				μg/kg PET	/kg PET	%
			<u> </u>			
	1-Heptanol, 2propyl-	C10H22O	10042-59-8	1024.59		100.0
	1-Heptanol, 2propyl- 1-Heptanol, 2propyl-	C10H22O C10H22O	10042-59-8 10042-59-8	1024.59 805.48		100.0 100.0
	1-Heptanol, 2propyl-	C10H22O	10042-59-8	805.48		100.0
	1-Heptanol, 2propyl- Nonanal	C10H22O C9H18O	10042-59-8 124-19-6	805.48 471.70		100.0 100.0
0	1-Heptanol, 2propyl- Nonanal 1-Dodecanol	C10H22O C9H18O C12H26O	10042-59-8 124-19-6 112-53-8	805.48 471.70 402.82		100.0 100.0 100.0
E 10	1-Heptanol, 2propyl- Nonanal 1-Dodecanol D-Limonene	C10H22O C9H18O C12H26O C10H16	10042-59-8 124-19-6 112-53-8 5989-27-5	805.48 471.70 402.82 132.19		100.0 100.0 100.0 100.0
APLE 10	1-Heptanol, 2propyl- Nonanal 1-Dodecanol D-Limonene Ethanol, 2-(2butoxyethoxy)-	C10H22O C9H18O C12H26O C10H16 C8H18O3	10042-59-8 124-19-6 112-53-8 5989-27-5 112-34-5	805.48 471.70 402.82 132.19 84.37	1033.58	100.0 100.0 100.0 100.0 100.0
SAMPLE 10	1-Heptanol, 2propyl- Nonanal 1-Dodecanol D-Limonene Ethanol, 2-(2butoxyethoxy)- Cyclohexanol, 2-(1,1-dimethylethyl)-, acetate	C10H22O C9H18O C12H26O C10H16 C8H18O3 C12H22O2	10042-59-8 124-19-6 112-53-8 5989-27-5 112-34-5 20298-69-5	805.48 471.70 402.82 132.19 84.37	1033.58 671.97	100.0 100.0 100.0 100.0 100.0
SAMPLE 10	1-Heptanol, 2propyl- Nonanal 1-Dodecanol D-Limonene Ethanol, 2-(2butoxyethoxy)- Cyclohexanol, 2-(1,1-dimethylethyl)-, acetate 2-Butenal, (Z)-	C10H22O C9H18O C12H26O C10H16 C8H18O3 C12H22O2 C4H6O	10042-59-8 124-19-6 112-53-8 5989-27-5 112-34-5 20298-69-5 15798-64-8	805.48 471.70 402.82 132.19 84.37		100.0 100.0 100.0 100.0 100.0
SAMPLE 10	1-Heptanol, 2propyl- Nonanal 1-Dodecanol D-Limonene Ethanol, 2-(2butoxyethoxy)- Cyclohexanol, 2-(1,1-dimethylethyl)-, acetate 2-Butenal, (Z)- 2,4-Hexadiene, 2,5dimethyl-	C10H22O C9H18O C12H26O C10H16 C8H18O3 C12H22O2 C4H6O C8H14	10042-59-8 124-19-6 112-53-8 5989-27-5 112-34-5 20298-69-5 15798-64-8 764-13-6	805.48 471.70 402.82 132.19 84.37	671.97	100.0 100.0 100.0 100.0 100.0 100.0
SAMPLE 10	1-Heptanol, 2propyl- Nonanal 1-Dodecanol D-Limonene Ethanol, 2-(2butoxyethoxy)- Cyclohexanol, 2-(1,1-dimethylethyl)-, acetate 2-Butenal, (Z)- 2,4-Hexadiene, 2,5dimethyl- 2,4-Hexadiene, 3,4dimethyl-,	C10H22O C9H18O C12H26O C10H16 C8H18O3 C12H22O2 C4H6O C8H14 C8H14	10042-59-8 124-19-6 112-53-8 5989-27-5 112-34-5 20298-69-5 15798-64-8 764-13-6 2417-88-1	805.48 471.70 402.82 132.19 84.37	671.97 789.95	100.0 100.0 100.0 100.0 100.0
SAMPLE 10	1-Heptanol, 2propyl- Nonanal 1-Dodecanol D-Limonene Ethanol, 2-(2butoxyethoxy)- Cyclohexanol, 2-(1,1-dimethylethyl)-, acetate 2-Butenal, (Z)- 2,4-Hexadiene, 2,5dimethyl- 2,4-Hexadiene, 3,4dimethyl-, Dipropylene glycol Dipropylene glycol Dipropylene glycol	C10H22O C9H18O C12H26O C10H16 C8H18O3 C12H22O2 C4H6O C8H14 C8H14	10042-59-8 124-19-6 112-53-8 5989-27-5 112-34-5 20298-69-5 15798-64-8 764-13-6 2417-88-1 110-98-5	805.48 471.70 402.82 132.19 84.37	671.97 789.95 4765.67	100.0 100.0 100.0 100.0 100.0
SAMPLE 10	1-Heptanol, 2propyl- Nonanal 1-Dodecanol D-Limonene Ethanol, 2-(2butoxyethoxy)- Cyclohexanol, 2-(1,1-dimethylethyl)-, acetate 2-Butenal, (Z)- 2,4-Hexadiene, 2,5dimethyl- 2,4-Hexadiene, 3,4dimethyl-, Dipropylene glycol Dipropylene glycol	C10H22O C9H18O C12H26O C10H16 C8H18O3 C12H22O2 C4H6O C8H14 C8H14 C6H14O3 C6H14O3	10042-59-8 124-19-6 112-53-8 5989-27-5 112-34-5 20298-69-5 15798-64-8 764-13-6 2417-88-1 110-98-5 110-98-5	805.48 471.70 402.82 132.19 84.37	671.97 789.95 4765.67 3062.13	100.0 100.0 100.0 100.0 100.0 - - -

Non Volatiles

	RT	Mass	Candidate	Formula	Input μg/kg PET	Output µg/kg PET	Cleaning efficiency, %
	5.84	429.1187	Cyclic TPA2-EG-DEG	C22H20O9	210	164	21.9
	6.71		Cyclic (TPA-EG)3	C30H24O12	187	281	-50.3
-	6.57		Cyclic (TPA3-EG2-DEG)	C32H28O13	88	65.6 40.6	25.5
SAMPLE	5.77 6.31	473.1453 385.0922	Cyclic (TPA-DEG)2	C24H24O10	39.9 24.5	30.7	-1.8 -25.3
₹	5.31		Cyclic (TPA-EG)2 (TPA-DEG)2+H2O	C20H16O8	21.3	16.6	-25.3 22.1
Ň	6.85	835.1853	Cyclic (TPA4-EG3DEG)	Fragment of 425.0843 m/z C20H18O9 C42H36O17	17.4	20.5	-17.8
	6.11		(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O13	14.3	13.8	3.5
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	12	21.2	-76.7
	3.50	002.2333	This Ede Section	5215027			76.7
	RT	Mass	Candidate	Formula	Input μg/kg PET	Output µg/kg PET	Cleaning efficiency, %
	6.71	577.1345	Cyclic (TPA-EG)3	C30H24O12	273	117	57.1
	5.84		Cyclic TPA2-EG-DEG	C22H20O9	268	359	-34.0
~	6.57		Cyclic (TPA3-EG2-DEG)	C32H28O13	129	186	-44.2
Ë	6.31		Cyclic (TPA-EG)2	C20H16O8	40.5		100.0
SAMPLE 2	6.82		Cyclic NPG-TPA-NPG-TPA	C26H28O8	40	25.7	35.8
SA	5.77		Cyclic (TPA-DEG)2	C24H24O10	34.3	49.2	-43.4
	6.11		(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O13	26.2		100.0
	5.98		TPA3-EG2-DEG+H2O (TPA-DEG)2+H2O	C32H30O14	25.6		100.0 100.0
	5.51	363.0913	(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	21.3		100.0
	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
	6.57	621.1603	Cyclic (TPA3-EG2-DEG)	C32H28O13	355	405	-14.1
	5.84	429.1187	Cyclic TPA2-EG-DEG	C22H20O9	254	255	-0.4
	6.11	577.1339	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O13	139	124	10.8
SAMPLE 3	6.31	385.0922	Cyclic (TPA-EG)2	C20H16O8	104	120	-15.4
₹	5.77	473.1453	Cyclic (TPA-DEG)2	C24H24O10	39	51.5	-32.1
SA	6.71		Cyclic (TPA-EG)3	C30H24O12	28.4	31.1	-9.5
	6.82	469.1854	Cyclic NPG-TPA-NPG-TPA	C26H28O8	23.6	25.3	-7.2
I							
	5.31		(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	22.7	0	100.0
		385.0915 661.1533	(TPA-DEG)2+H2O TPA3-EG2-DEG+H2O	Fragment of 425.0843 m/z C20H18O9 C32H30O14	22.7 16.3		100.0 -8.0
	5.31 5.98 RT	661.1533 Mass	TPA3-EG2-DEG+H2O Candidate	C32H30O14 Formula	16.3 Input μg/kg PET	0 17.6 Output µg/kg PET	-8.0 Cleaning efficiency, %
	5.31 5.98 RT	Mass 429.1187	TPA3-EG2-DEG+H2O Candidate Cíclico TPA2-EG-DEG	C32H30O14 Formula C22H20O9	Input µg/kg PET 215	0 17.6 Output µg/kg PET	-8.0 Cleaning efficiency, %
	5.31 5.98 RT 5.84 6.71	Mass 429.1187 577.1345	TPA3-EG2-DEG+H2O Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3	C32H30O14 Formula C22H20O9 C30H24O12	Input µg/kg PET 215 184	0 17.6 Output µg/kg PET 230 166	-8.0 Cleaning efficiency, % -7.0 9.8
4	5.31 5.98 RT 5.84 6.71 6.57	Mass 429.1187 577.1345 621.1603	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA3-EG2DEG)	C32H30O14 Formula C22H20O9 C30H24O12 C32H28O13	16.3 Input µg/kg PET 215 184 93.6	0 17.6 Output μg/kg PET 230 166 92.7	-8.0 Cleaning efficiency, % -7.0 9.8 1.0
PLE 4	5.31 5.98 RT 5.84 6.71 6.57 5.77	Mass 429.1187 577.1345 621.1603 473.1453	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA3-EG2DEG) Cíclico (TPA-DEG)2	C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010	16.3 Input µg/kg PET 215 184 93.6 48.8	0 17.6 Output μg/kg PET 230 166 92.7 65.3	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8
AMPLE 4	5.31 5.98 RT 5.84 6.71 6.57 5.77 6.85	Mass 429.1187 577.1345 621.1603 473.1453 835.1853	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA3-EG2DEG) Cíclico (TPA-DEG)2 Cyclic (TPA4-EG3DEG)	C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017	Input µg/kg PET 215 184 93.6 48.8 22.1	0 17.6 Output μg/kg PET 230 166 92.7 65.3	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7
SAMPLE 4	5.31 5.98 RT 5.84 6.71 6.57 5.77 6.85 6.31	Mass 429.1187 577.1345 621.1603 473.1453 835.1853 385.0922	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA-EG2DEG) Cíclico (TPA-DEG)2 Cyclic (TPA4-EG3DEG) Cíclico (TPA-EG)2	C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608	Input μg/kg PET 215 184 93.6 48.8 22.1 21.4	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9
SAMPLE 4	5.31 5.98 RT 5.84 6.71 6.57 5.77 6.85 6.31 5.31	Mass 429.1187 577.1345 621.1603 473.1453 835.1853 385.0922 385.0915	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA-EG2DEG) Cíclico (TPA-DEG)2 Cyclic (TPA4-EG3DEG) Cíclico (TPA-EG)2 (TPA-DEG)2 (TPA-DEG)2+H2O	C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608 Fragment of 425.0843 m/z C20H1809	Input μg/kg PET 215 184 93.6 48.8 22.1 21.4 19.5	0 17.6 Output μg/kg PET 230 166 92.7 65.3	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 40.5
SAMPLE 4	5.31 5.98 RT 5.84 6.71 6.57 5.77 6.85 6.31 5.31	Mass 429.1187 577.1345 621.1603 473.1453 835.1853 385.0922 385.0915 577.1339/	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA3-EG2DEG) Cíclico (TPA-DEG)2 Cyclic (TPA4-EG3DEG) Cíclico (TPA-EG)2 (TPA-DEG)2 (TPA-DEG)2+H2O (TPA-EG)3+H2O	C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608 Fragment of 425.0843 m/z C20H1809 Fragment of 617.1263 m/z C30H2601:	Input μg/kg PET 215 184 93.6 48.8 22.1 21.4	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8 11.6	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 40.5
SAMPLE 4	5.31 5.98 RT 5.84 6.71 6.57 6.85 6.31 5.31 6.11	Mass 429.1187 577.1345 621.1603 473.1453 835.1853 385.0922 385.0915 577.1339/	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA-EG2DEG) Cíclico (TPA-DEG)2 Cyclic (TPA4-EG3DEG) Cíclico (TPA-EG)2 (TPA-DEG)2 (TPA-DEG)2+H2O	C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608 Fragment of 425.0843 m/z C20H1809	Input µg/kg PET 215 184 93.6 48.8 22.1 21.4 19.5	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 40.5 100.0
SAMPLE 4	5.31 5.98 RT 5.84 6.71 6.57 6.85 6.31 5.31 6.11	Mass 429.1187 577.1345 621.1603 473.1453 835.1853 385.0922 385.0915 577.1339/ 661.1533	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA3-EG2DEG) Cíclico (TPA-EG)2 Cyclic (TPA4-EG3DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG)2 (TPA4-EG)2+H2O (TPA-EG)2+H2O (TPA-EG)3+H2O TPA3-EG2-DEG+H2O Candidate	C32H30O14 Formula C22H20O9 C30H24O12 C32H28O13 C24H24O10 C42H36O17 C20H16O8 Fragment of 425.0843 m/z C20H18O9 Fragment of 617.1263 m/z C30H26O1: C32H30O14 Formula	Input μg/kg PET 215 184 93.6 48.8 22.1.4 19.5 14.9 13 Input μg/kg PET	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8 11.6 9.8	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 40.5 100.0 24.6 Cleaning efficiency, %
SAMPLE 4	5.31 5.98 RT 5.84 6.71 6.57 5.77 6.85 6.31 6.11 5.98	Mass 429.1187 577.1345 621.1603 473.1453 835.1853 385.0922 385.0915 577.1339/ 661.1533 Mass 429.1187	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA3-EG2DEG) Cíclico (TPA-EG)2 Cyclic (TPA4-EG3DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG)2 (TPA4-EG)2 (TPA4-EG)2+H2O (TPA4-EG)3+H2O TPA3-EG2-DEG+H2O Candidate Cíclico TPA2-EG-DEG	C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608 Fragment of 425.0843 m/z C20H1809 Fragment of 617.1263 m/z C30H2601: C32H30014 Formula C22H2009	Input µg/kg PET 215 184 93.6 48.8 22.1 21.4 19.5 14.9 13 Input µg/kg PET 237	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8 9.8 Output μg/kg PET 231	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 40.5 100.0 24.6 Cleaning efficiency, %
SAMPLE 4	5.31 5.98 RT 5.84 6.71 6.57 5.77 6.85 6.31 5.98 RT 5.84 6.71	Mass 429.1187 577.1345 621.1603 473.1453 835.1853 385.0912 577.1339/ 661.1533 Mass 429.1187 577.1345	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA3-EG2DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG3CAC) CÍCPA4-EG3+H2O TPA3-EG2-DEG+H2O Candidate Cíclico TPA2-EG-DEG Cíclico (TPA4-EG)3	C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608 Fragment of 425.0843 m/z C20H1809 Fragment of 617.1263 m/z C30H2601: C32H30014 Formula C22H2009 C30H24012	Input µg/kg PET 215 184 93.6 48.8 22.1 21.4 19.5 14.9 13 Input µg/kg PET 237 144	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8 11.6 9.8 Output μg/kg PET 231 141	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 40.5 100.0 24.6 Cleaning efficiency, %
SAMPLE	5.31 5.98 RT 5.84 6.71 6.57 5.77 6.85 6.31 5.31 6.51 5.98 RT 5.84 6.71 6.57	Mass 429.1187 577.1345 621.1603 473.1453 835.1853 385.0912 385.0915 577.1339/ 661.1533 Mass 429.1187 577.1345 621.1603	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA3-EG2DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG3DEG) Cíclico (TPA4-EG)2 (TPA-EG)2 (TPA-EG)3+H2O TPA3-EG2-DEG+H2O Candidate Cíclico TPA2-EG-DEG Cíclico (TPA4-EG)3 Cíclico (TPA3-EG2DEG)	Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608 Fragment of 425.0843 m/z C20H1809 Fragment of 617.1263 m/z C30H2601: C32H30014 Formula C22H2009 C30H24012 C32H28013	Input µg/kg PET 215 184 93.6 48.8 22.1 21.4 19.5 14.9 13 Input µg/kg PET 237 144 83.2	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8 11.6 9.8 Output μg/kg PET 231 141 90.4	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 40.5 100.0 24.6 Cleaning efficiency, % 2.5 2.1
SAMPLE	5.31 5.98 RT 5.84 6.71 6.57 6.85 6.31 5.31 6.11 5.98 RT 5.84 6.71 6.57 5.77	Mass 429.1187 577.1345 621.1603 473.1453 385.0915 577.1339/ 661.1533 Mass 429.1187 577.1345 621.1603 473.1453	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA-EG)2 Cýclic (TPA-EG)2 Cýclic (TPA-EG)2 Cíclico (TPA-EG)2 (TPA-DEG)2 (TPA-DEG)2+H2O (TPA-EG)3+H2O TPA3-EG2-DEG+H2O Cíclico TPA2-EG-DEG Cíclico (TPA2-EG-DEG) Cíclico (TPA3-EG2-DEG) Cíclico (TPA3-EG2-DEG) Cíclico (TPA3-EG3-DEG) Cíclico (TPA3-EG3-DEG) Cíclico (TPA3-EG3-DEG) Cíclico (TPA3-EG3-DEG) Cíclico (TPA3-EG3-DEG)	Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608 Fragment of 425.0843 m/z C20H1809 Fragment of 617.1263 m/z C30H2601: C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010	Input µg/kg PET 215 184 93.6 48.8 22.1 21.4 19.5 14.9 13 Input µg/kg PET 237 144 83.2 42.8	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8 11.6 9.8 Output μg/kg PET 231 141 90.4 63.2	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 40.5 100.0 24.6 Cleaning efficiency, % 2.5 2.1 -8.7 -47.7
SAMPLE	5.31 5.98 RT 5.84 6.71 6.57 5.77 6.85 6.31 5.31 6.11 5.98 RT 5.84 6.71 6.57 5.77 6.57	Mass 429.1187 577.1345 621.1603 473.1453 385.0912 385.0915 577.1339/ 661.1533 Mass 429.1187 577.1345 621.1603 473.1453 385.0922	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA-EG)2 Cýclic (TPA-EG)2 Cýclic (TPA-EG)2 Cíclico (TPA-EG)2 (TPA-DEG)2 (TPA-DEG)2+H2O (TPA-EG)3+H2O TPA3-EG2-DEG+H2O Cíclico TPA2-EG-DEG Cíclico (TPA2-EG)3 Cíclico (TPA2-EG)3 Cíclico (TPA3-EG2-DEG) Cíclico (TPA3-EG2-DEG) Cíclico (TPA3-EG3-DEG)	Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608 Fragment of 425.0843 m/z C20H1809 Fragment of 617.1263 m/z C30H2601: C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010 C20H1608	Input µg/kg PET 215 184 93.6 48.8 22.1 21.4 19.5 14.9 13 Input µg/kg PET 237 144 83.2 42.8 24.3	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8 11.6 9.8 Output μg/kg PET 231 141 90.4 63.2 27.8	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 40.5 100.0 24.6 Cleaning efficiency, % 2.5 2.1 -8.7 -47.7 -14.4
SAMPLE 5 SAMPLE 4	5.31 5.98 RT 5.84 6.71 6.57 5.77 6.85 6.31 5.31 6.11 5.98 RT 5.84 6.71 6.57 5.77 6.57 5.77	Mass 429.1187 577.1345 621.1603 473.1453 385.0912 385.0915 577.1339/ 661.1533 Mass 429.1187 577.1345 621.1603 473.1453 385.0922 385.0915	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA3-EG2DEG) Cíclico (TPA-EG)2 Cyclic (TPA4-EG3DEG) Cíclico (TPA-EG)2 (TPA-DEG)2+H2O (TPA-EG)3+H2O TPA3-EG2-DEG+H2O Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA-EG)3 Cíclico (TPA-EG)3 Cíclico (TPA-EG)3 Cíclico (TPA-EG)3 Cíclico (TPA-EG)3 Cíclico (TPA-EG)2	Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608 Fragment of 425.0843 m/z C20H1809 Fragment of 617.1263 m/z C30H26012 C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010 C20H1608 Fragment of 425.0843 m/z C20H1809	Input µg/kg PET 215 184 93.6 48.8 22.1 21.4 19.5 14.9 13 Input µg/kg PET 237 144 83.2 42.8 24.3 21.4	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8 11.6 9.8 Output μg/kg PET 231 141 90.4 63.2 27.8 16.8	Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 40.5 100.0 24.6 Cleaning efficiency, % 2.5 -8.7 -47.7 -14.4 21.5
SAMPLE	5.31 5.98 RT 5.84 6.71 6.57 5.77 6.85 6.31 5.31 6.11 5.98 RT 5.84 6.71 6.57 5.77 6.57	Mass 429.1187 577.1345 621.1603 473.1453 385.0921 577.1339/ 661.1533 Mass 429.1187 577.1345 621.1603 473.1453 385.0922 385.0915 835.1853	Candidate Cíclico TPA2-EG-DEG Cíclico (TPA-EG)3 Cíclico (TPA-EG)2 Cýclic (TPA-EG)2 Cýclic (TPA-EG)2 Cíclico (TPA-EG)2 (TPA-DEG)2 (TPA-DEG)2+H2O (TPA-EG)3+H2O TPA3-EG2-DEG+H2O Cíclico TPA2-EG-DEG Cíclico (TPA2-EG)3 Cíclico (TPA2-EG)3 Cíclico (TPA3-EG2-DEG) Cíclico (TPA3-EG2-DEG) Cíclico (TPA3-EG3-DEG)	Formula C22H2009 C30H24012 C32H28013 C24H24010 C42H36017 C20H1608 Fragment of 425.0843 m/z C20H1809 Fragment of 617.1263 m/z C30H2601: C32H30014 Formula C22H2009 C30H24012 C32H28013 C24H24010 C20H1608	Input µg/kg PET 215 184 93.6 48.8 22.1 21.4 19.5 14.9 13 Input µg/kg PET 237 144 83.2 42.8 24.3	0 17.6 Output μg/kg PET 230 166 92.7 65.3 14 11.8 11.6 9.8 Output μg/kg PET 231 141 90.4 63.2 27.8	-8.0 Cleaning efficiency, % -7.0 9.8 1.0 -33.8 36.7 44.9 100.0 24.6 Cleaning efficiency, %

Non Volatiles (contd)

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
	6.71		Cyclic (TPA-EG)3	C30H24O12	341	342	-0.3
	5.84		Cyclic TPA2-EG-DEG	C22H20O9	282	655	-132.3
9	6.57		Cyclic (TPA3-EG2-DEG)	C32H28O13	126	223	-77.0
SAMPLE 6	5.77		Cyclic (TPA-DEG)2	C24H24O10	50.6 42.8	114 60.3	-125.3
¥	6.85 5.31		Cyclic (TPA4-EG3DEG) (TPA-DEG)2+H2O	C42H36O17 Fragment of 425.0843 m/z C20H18O9	39	73.2	-40.9 -87.7
S	6.31		Cyclic (TPA-EG)2	C20H16O8	37.5	23.7	36.8
	5.98		TPA3-EG2-DEG+H2O	C32H30O14	31	61.5	-98.4
	6.11	577.1339/	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	30.9	34.3	-11.0
			, <u></u>				
	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
	6.71		Cyclic (TPA-EG)3	C30H24O12	541	425	21.4
	5.84		Cyclic TPA2-EG-DEG	C22H20O9	377	303	19.6
7	6.31		Cyclic (TPA-EG)2	C20H16O8	252	190	24.6
FE.	6.57		Cyclic (TPA3-EG2-DEG)	C32H28O13	155 61.9	130 52	16.1
SAMPLE 7	5.77		Cyclic (TPA-DEG)2 Cyclic NPG-TPA-NPG-TPA	C24H24O10 C26H28O8	40	25.7	16.0 35.8
S	6.82 5.31		(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	29.2	25.7	100.0
	5.98		TPA3-EG2-DEG+H2O	C32H30O14	27.1	20.4	24.7
	6.11	577.1339	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	25.8	20.7	100.0
	0.11	377.12333	(IIII Edjalliza	Tragillation of the state of th	23.0		200.0
	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	
	5.84		Cyclic TPA2-EG-DEG	C22H20O9	391	497	-27.1
	6.71		Cyclic (TPA-EG)3	C30H24O12	340	327	3.8
00	6.57		Cyclic (TPA3-EG2-DEG)	C32H28O13	149	166	-11.4
SAMPLE 8	5.77 6.85		Cyclic (TPA-DEG)2 Cyclic NPG-TPA-NPG-TPA	C24H24O10	58.6 52.6	67.7 48.4	-15.5 8.0
Σ	6.31		Cyclic (TPA-EG)2	C42H36O17 C20H16O8	45.2	37.5	17.0
Š	6.11		(TPA-EG)2	Fragment of 617.1263 m/z C30H26O1	44.7	19.6	56.2
	5.98		TPA3-EG2-DEG+H2O	C32H30O14	38.3	36.7	4.2
	5.31		(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	34.7	36	-3.7
	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	-
	6.71		Cyclic (TPA-EG)3	C30H24O12	251	211	15.9
E 9	5.84		Cyclic TPA2-EG-DEG	C22H20O9	173	174	-0.6
SAMPLE 9	6.57	621.1603 385.0922	Cyclic (TPA3-EG2-DEG) Cyclic (TPA-EG)2	C32H28O13	83.9 59.2	44.4 107	47.1 -80.7
SAR	6.31 5.77	473.1453	Cyclic (TPA-EG)2	C20H16O8 C24H24O10	25.8	25.9	-80.7
	5.98		TPA3-EG2-DEG+H2O	C32H30O14	19.3	22.9	-18.7
	3.30	001.1333	117A3-E02-DEG11120	C321130014	15.5	22.5	-10.7
	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
	6.71	577.1345	Cyclic (TPA-EG)3	C30H24O12	242	274	-13.2
	5.84		Cyclic TPA2-EG-DEG	C22H20O9	220	272	-23.6
9	6.57		Cyclic (TPA3-EG2-DEG)	C32H28O13	99.2	114	-14.9
SAMPLE 10	6.31		Cyclic (TPA-EG)2	C20H16O8	37.2	0	100.0
₫	5.77		Cyclic (TPA-DEG)2	C24H24O10	34.4	42.4	-23.3
SA	5.31		(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H1809	21.9	12.9	41.1
	6.11		(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	18.2	10.8	40.7
	5.98		TPA3-EG2-DEG+H2O	C32H30O14	14.9	9.06	39.2
	6.82	469.1854	Cyclic NPG-TPA- NPG-TPA	C26H28O8		512	-

Inorganic Substances

	Substance	INPUT mg/Kg of PET	OUTPUT mg/Kg of PET	LOD		Substance	INPUT mg/Kg of PET	OUTPUT mg/Kg of PET	LOD
	Cr	8.57	\	0.06]	Cr	0.15	0.55	0.06
_	Mn	0.45	0.2	0.04		Mn	0.15	0.14	0.04
7	Fe	20.28	5.72	1.37	9	Fe	N/A	2.66	1.37
SAMPLE	Co	2.36	1.11	0.01	SAMPLE	Co	0.05	0.11	0.01
Ь	Ni	2.99	1.85	0.32		Ni	1.08	1.41	0.32
Σ	Zn	N/A	N/A	6.4	- ≥	Zn	N/A	N/A	6.4
₹	Ge	0.3	0.39	0.03	₹	Ge	0.25	0.27	0.03
S	As Zr	N/A	0.05	0.02	S	As Zr	N/A	1.06	0.02
	Ba	N/A	4.91	0.02	1	Ba	0.77	2.56	0.02
	Sb	171.10	170.60	0.03	1	Sb	199.74	211.03	0.03
	Se	N/A	N/A	3.6	1	Se	N/A	N/A	3.6
	Pb	N/A	4.4	0.51	1	Pb	0.83	2.41	0.51
	Substance	INPUT	OUTPUT	LOD		Substance	INPUT	OUTPUT	LOD
	Cr	0.1	0.23	0.06		Cr	0.6	N/A	0.06
	Mn	0.62	0.64	0.04	1	Mn	0.4	0.31	0.04
7	Fe	8.3	7.45	1.37	_	Fe	8.56	N/A	1.37
ш	Co	0.09	0.83	0.01	ш	Co	1.88	1.03	0.01
Ž	Ni Zn	1.39 N/A	0.77 N/A	0.32 6.4		Ni Zn	2.01 N/A	1 N/A	0.32 6.4
4	Ge	0.26	1	0.03		Ge	0.22	0.25	0.03
2	As	0.04	0.09	0.02	2	As	0.05	0.04	0.02
SAMPLE	Zr	N/A	N/A	0.02	SAMPLE	Zr	N/A	N/A	0.02
9)	Ba	N/A	N/A	0.15	٠,	Ba	1.71	N/A	0.15
	Sb	193.20	179.82	0.03		Sb	205.18	174.80	0.03
	Se	N/A	N/A	3.6	1	Se	N/A	N/A	3.6
	Pb	N/A	N/A	0.51	-	Pb	1.65	N/A	0.51
	Substance Cr	0.26	OUTPUT 1.73	0.06	1	Substance Cr	1NPUT 0.71	OUTPUT <lod< th=""><th>0.06</th></lod<>	0.06
	Mn	0.20	0.14	0.04	1	Mn	0.50	0.11	0.04
	Fe	6.92	4.28	1.37		Fe	15.2	5.29	1.37
m	Co	1.01	0.68	0.01	∞ ×	Co	0.62	0.37	0.01
Щ	Ni	1.04	1.35	0.32	Щ	Ni	1.74	1.07	0.32
SAMPLE 3	Zn	N/A	N/A	6.4	SAMPLE	Zn	<lod< td=""><td><lod< td=""><td>6.4</td></lod<></td></lod<>	<lod< td=""><td>6.4</td></lod<>	6.4
5	Ge	0.54	0.49	0.03	>	Ge	0.26	0.24	0.03
A	As Zr	0.06	0.07	0.02	₹	As	0.05	0.03	0.02
S	Ba	3.8	N/A N/A	0.02	S	Zr Ba	1.56 5.39	<lod <lod< td=""><td>0.02 0.15</td></lod<></lod 	0.02 0.15
	Sb	189.70	193.08	0.03	1	Sb	198.93	225.52	0.03
	Se	N/A	N/A	3.6	1	Se	<lod< td=""><td><lod< td=""><td>3.6</td></lod<></td></lod<>	<lod< td=""><td>3.6</td></lod<>	3.6
	Pb	2.7	N/A	0.51	1	Pb	5.02	<lod< th=""><th>0.51</th></lod<>	0.51
	Substance	INPUT	OUTPUT	LOD		Substance	INPUT	OUTPUT	LOD
	Cr	0.09				~			
	Mn		1.54	0.06	1	Cr	N/A	N/A	0.06
		0.38	0.17	0.04		Mn	N/A	N/A	0.04
4	Fe	2.1	0.17 1.55	0.04 1.37	6	Mn Fe	N/A N/A	N/A N/A	0.04 1.37
	Co	2.1 0.97	0.17 1.55 0.93	0.04 1.37 0.01		Mn Fe Co	N/A N/A N/A	N/A N/A N/A	0.04 1.37 0.01
Щ	Co Ni	2.1 0.97 0.83	0.17 1.55 0.93 1.41	0.04 1.37 0.01 0.32	"	Mn Fe Co Ni	N/A N/A N/A N/A	N/A N/A N/A	0.04 1.37 0.01 0.32
Щ	Co	2.1 0.97	0.17 1.55 0.93	0.04 1.37 0.01	"	Mn Fe Co	N/A N/A N/A	N/A N/A N/A	0.04 1.37 0.01
Щ	Co Ni Zn	2.1 0.97 0.83 N/A	0.17 1.55 0.93 1.41 N/A	0.04 1.37 0.01 0.32 6.4	"	Mn Fe Co Ni Zn	N/A N/A N/A N/A	N/A N/A N/A N/A	0.04 1.37 0.01 0.32 6.4
Щ	Co Ni Zn Ge As Zr	2.1 0.97 0.83 N/A 0.37 0.06 N/A	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02	"	Mn Fe Co Ni Zn Ge As Zr	N/A N/A N/A N/A N/A N/A N/A	N/A N/A N/A N/A N/A N/A N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02
	Co Ni Zn Ge As Zr	2.1 0.97 0.83 N/A 0.37 0.06 N/A	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02		Mn Fe Co Ni Zn Ge As Zr Ba	N/A N/A N/A N/A N/A N/A N/A N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02
Щ	Co Ni Zn Ge As Zr Ba Sb	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15	"	Mn Fe Co Ni Zn Ge As Zr Ba Sb	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15
Щ	Co Ni Zn Ge As Zr Ba Sb Se	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6	"	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6
Щ	Co Ni Zn Ge As Zr Ba Sb Se	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6	"	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6
Щ	Co Ni Zn Ge As Zr Ba Sb Se	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6	"	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6
Щ	Co Ni Zn Ge As Zr Ba Sb Se Pb Substance	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A N/A INPUT	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A N/A OUTPUT	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51	"	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se Pb Substance	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.05 0.03 3.6 0.51
SAMPLE	Co Ni Zn Ge As Zr Ba Sb Sc Pb Substance	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A N/A INPUT 1.3	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A OUTPUT 4.6	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD	SAMPLE	Mn Fe Co Ni Zn Ge As Zr Ba Sb Sb Se Pb Substance Cr	N/A	N/A	0.04 1.37 0.01 0.32 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD
SAMPLE	Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A N/A INPUT 1.3 0.41 8.8 1.01	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A N/A OUTPUT 4.6 0.44 12.67 0.53	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01	SAMPLE	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01
SAMPLE	Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A N/A INPUT 1.3 0.41 8.8 1.01 1.64	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A 200.63 N/A N/A OUTPUT 4.6 0.44 12.67 0.53 2.75	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32	SAMPLE	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32
SAMPLE	Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni Zn	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A N/A INPUT 1.3 0.41 8.8 1.01 1.64 N/A	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A 200.63 N/A N/A OUTPUT 4.6 0.44 12.67 0.53 2.75 N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32 6.4	SAMPLE	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni Zn	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32 6.4
SAMPLE	Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni Zn Ge	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A N/A INPUT 1.3 0.41 8.8 1.01 1.64 N/A	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A N/A OUTPUT 4.6 0.44 12.67 0.53 2.75 N/A 0.31	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32 6.4 0.03	SAMPLE	Mn Fe Co Ni Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni Zn Ge	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32 6.4 0.03
SAMPLE	Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni Zn Ge As	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A INPUT 1.3 0.41 8.8 1.01 1.64 N/A	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A OUTPUT 4.6 0.44 12.67 0.53 2.75 N/A 0.31	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.03 2.6.4 0.03 0.02	SAMPLE	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni Zn Ge As	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32 6.4 0.03 0.02
Щ	Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni Zn Ge As Zr	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A N/A INPUT 1.3 0.41 8.8 1.01 1.64 N/A 0.34	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A OUTPUT 4.6 0.44 12.67 0.53 2.75 N/A 0.31 0.03 N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32 6.4 0.03 0.02	"	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se Cr Mn Fe Co Ni Substance Cr Mn Fe Co Ni Zn	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02
SAMPLE	Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni Zn Ge As	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A N/A INPUT 1.3 0.41 8.8 1.01 1.64 N/A 0.34 0.04	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A N/A OUTPUT 4.6 0.44 12.67 0.53 2.75 N/A 0.31 0.03 N/A N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.03 2.6.4 0.03 0.02	SAMPLE	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni Zn Ge As	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32 6.4 0.03 0.02
SAMPLE	Co Ni Zn Ge As Sb Se Pb Substance Cr Mn Fe Co Ni Zn Ge	2.1 0.97 0.83 N/A 0.37 0.06 N/A N/A 181.99 N/A N/A INPUT 1.3 0.41 8.8 1.01 1.64 N/A 0.34	0.17 1.55 0.93 1.41 N/A 0.59 0.11 N/A N/A 200.63 N/A OUTPUT 4.6 0.44 12.67 0.53 2.75 N/A 0.31 0.03 N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.02 0.15	SAMPLE	Mn Fe Co Ni Zn Ge As Zr Ba Sb Se Pb Substance Cr Mn Fe Co Ni Zn Ge As Zr	N/A	N/A	0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.15 0.03 3.6 0.51 LOD 0.06 0.04 1.37 0.01 0.32 6.4 0.03 0.02 0.15

Primary Aromatic Amines

Primary Aromatic Amines were not detected in the Input or Output samples.

No	Analyte	Name	CAS	LOQ (µg/Kg PET)	Sample pellets
1	p-PDA	<i>p</i> -Fenilendiamina	106-50-3	79.8	<loq< td=""></loq<>
2	m-PDA	<i>m</i> - Fenilendiamina	108-45-2	79.8	<loq< td=""></loq<>
3	2,6-TDA	2,6-Toluendiamina	823-40-5	14.6	<loq< td=""></loq<>
4	4-M-m-PDA	4-Methoxy- <i>m</i> - phenylenediamine	615-05-4	14.6	<loq< td=""></loq<>
5	2,4-TDA	2,4-Toluendiamina	95-80-7	14.6	<loq< td=""></loq<>
6	1,5-DAN	1,5-Diaminonaftaleno	2243-62-1	16.5	<loq< td=""></loq<>
7	ANL	Anilina	62-53-3	11.3	<loq< td=""></loq<>
8	BNZ	Bencidina	92-87-5	41.3	<loq< td=""></loq<>
9	o-ASD	o-Anisidina	90-04-0	99	<loq< td=""></loq<>
10	4,4-DPE	4,4-Oxidianilina	101-80-4	20.1	<loq< td=""></loq<>
11	o-T	o-Toluidina	95-53-4	33	<loq< td=""></loq<>
12	4-CA	4-Cloroanilina	106-47-8	33	<loq< td=""></loq<>
13	4,4-MDA	4,4-Metilenodianilina	101-77-9	21.5	<loq< td=""></loq<>
14	o-diASD	o-Dianisidina	119-90-4	3	<loq< td=""></loq<>
15	2-M-5-MA	2-Metoxi-5-m-toluidina	120-71-8	41.3	<loq< td=""></loq<>
16	3,3-DMB	3,3-Dimetilbencidina	119-93-7	17.9	<loq< td=""></loq<>
17	2,4-DMA	2,4-Dimetilanilina	87-62-7	3	<loq< td=""></loq<>
18	4,4'-thioANL	4,4'-Tiodianilina	139-65-1	71.5	<loq< td=""></loq<>
19	2,6-DMA	2,6-Dimetilanilina	95-68-1	3	<loq< td=""></loq<>
20	2-NA	2-Naftilamina	91-59-8	7.7	<loq< td=""></loq<>
21	4,4-MDoT	4,4-Metilenodi-o-toluidina	838-88-0	85.3	<loq< td=""></loq<>
22	4-ABP	4-Aminobifenilo	92-67-1	41.3	<loq< td=""></loq<>
23	4-AAB	4-Aminoazobenceno	60-09-3	17.3	<loq< td=""></loq<>
24	5-N-o-T	5-Nitro-o-toluidina	99-55-8	5.8	<loq< td=""></loq<>
25	1,4,5-TMA	2,4,5-Trimetilanilina	137-17-7	22	<loq< td=""></loq<>
26	4-CT	4-Cloro-o-toluidina	95-69-2	63.3	<loq< td=""></loq<>
27	AAT	o-Aminoazotolueno	97-56-3	5	<loq< td=""></loq<>
28	3,3-DCB	3,3-Diclorobencidina	91-94-1	129.3	<loq< td=""></loq<>
29	4,4-MCA	4,4-Metileno-bis-(2- cloroanilina)	101-14-4	4.4	<loq< td=""></loq<>

Plastics Additives

Plastics Additives Indicated in the following table were not detected in the Input or Output Samples

Additives	CAS	LOD (μg/Kg PET)	Results Input & Output
Irgafos 168	31570-04-4	LOD=110	<loq< td=""></loq<>
TopanolCA	1843-03-4	LOD=2750	<loq< td=""></loq<>
Chimassorb 81	1843-05-6	LOD=113	<loq< td=""></loq<>
Cyasorb UV 1084	14516-71-3	LOD=850	<loq< td=""></loq<>
Tinuvin 326	05/11/3896	LOD=157	<loq< td=""></loq<>
Irganox1010	6683-19-8	LOD=83	<loq< td=""></loq<>
Tinuvin 327	01/09/3864	LOD=270	<loq< td=""></loq<>
Irgafos 38	145650-60-8	LOD=570	<loq< td=""></loq<>
Irganox 1076	2082-79-3	LOD=725	<loq< td=""></loq<>
Tinuvin P	2440-22-4	LOD=2700	<loq< td=""></loq<>
9,9-bis (methoxymethyl) fluorene	182121-12-6	LOD=75	<loq< td=""></loq<>
N,N-Bis(2-hydroxyethyl)alkylamines (C12)	942-293-6	LOD=50	<loq< td=""></loq<>
Erucamide	112-84-5	LOD=193	<loq< td=""></loq<>
Bis(2-ethylhexyl) adipate	103-23-1	LOD=82	<loq< td=""></loq<>
Tributylcitrate	77-94-1	LOD=105	<loq< td=""></loq<>
Trybutyl o-acetylcitrate	77-90-7	LOD=75	<loq< td=""></loq<>
TXIB (2,2,4- Trimethyl-1,3- pentanedioldiisobutyrate)	6846-50-0	LOD=2600	<loq< td=""></loq<>
Bis(2-ethylhexyl) sebacate	122-62-3	LOD=52	<loq< td=""></loq<>
NX8000	882073-43-0	LOD=1650	<loq< td=""></loq<>

d) List of contaminating materials regularly present in the plastic input

Table 1 lists the contaminating materials regularly present in the plastic input.

Typical Residuals						
Property	Maximum	Units				
PVC	50	mg/kg				
Polyolefin (caps/labels)	20	mg/kg				
Other Polymers	100	mg/kg				
Metal	10	mg/kg				
Other Inert Materials	30	mg/kg				

Table 1. Contaminating materials regularly present in the plastic input.

e) Analysis of the most likely origin of the identified contaminants referred to in points (c) and (d).

Input material

Depending on the collection and sorting process, post-consumer PET waste can contain a limited amount of other polymers and materials such as polyolefins, polyvinyl Chloride (PVC), polyamide (PA), ethylene vinyl alcohol (EVOH), polystyrene (PS) and fillers. These polymers and materials originate from the following sources:

- Polyolefins like polyethylene (PE) and polypropylene (PP) are used to manufacture bottle closures and are present in a wide range of other plastic products.
- PVC is used in the manufacturing of certain labels and sleeves for bottles.
- PS is used in disposable cups and other packaging materials.
- EVOH is used as oxygen barrier in food packaging.
- PA is often used as barrier layer in flexible packaging films.
- Fillers are used in plastic packaging materials to modify their properties and enhance their performance.

The likely origin of the substances detected in the input material is as follows:

- Limonene: since a large fraction of PET bottles is used to pack flavoured beverages, the flavouring substance limonene is found in nearly all post-consumer PET waste streams (Franz *et al.*, 2004).
- Acetaldehyde: PET degradation product formed during injection moulding.

Output material

- Oligomers are generated during the PET Polymerisation Process.
- Acetaldehyde: PET degradation product formed during injection moulding

f) Measurement or estimation of the migration levels to food of contaminants present in the recycled plastic materials and articles.

Potential migration

Assuming worse case 100% of migration to food and considering that the average weight of PET of one litre PET bottle is 27.2g, the potential migration would be:

	Name	Formula	CAS	Output μg/kg PET	Potential Migration ug/Kg in food
SAMPLE 1	1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3	106-62-7	2170.85	59.05
	Dipropylene glycol	C6H14O3	110-98-5	2958.10	80.46
	1-Propanol, 2,2'oxybis-	C6H14O3	108-61-2	2525.77	68.70
	Nonanal	C9H18O	124-19-6	102.06	2.78
7	Dodecanal	C ₁₂ H ₂₄ O	112-54-9	87.58	2.38
SAMPLE 2	1,3-Dioxolane, 2-methyl-	C4H8O2	497-26-7	1997.90	54.34
Σ	Octanoic acid, ethyl ester	C10H20O2	106-32-1	44.69	1.22
Š	1-Undecanol	C11H24O	112-42-5	238.63	6.49
	Tetradecane	C14H30	629-59-4	46.90	1.28
	Ethanol, 2-(dodecyloxy)-	C14H30O2	4536-30-5	47.00	1.28
	Tetradecane	C14H30	629-59-4	87.84	2.39
m	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	6.14	0.17
SAMPLE 3	2-Propanol, 1,1'oxybis-	C6H14O3	110-98-5	2423.53	65.92
¥	Dipropylene glycol	C6H14O3	110-98-5	1528.43	41.57
S.	Dipropylene glycol	C6H14O3	110-98-5	2166.73	58.94
	7,9-Di-tert-butyl-oxaspiro(4,5)deca6,9-diene-2,8-dione	C ₁₇ H ₂₄ O ₃	82304-66-3	25.03	0.68
	n-Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	57-10-3	10.00	0.27
	Dipropylene glycol	C6H14O3	110-98-5	1732.47	47.12
	Dipropylene glycol	C6H14O3	110-98-5	1199.75	32.63
4	Dipropylene glycol	C6H14O3	110-98-5	1703.76	46.34
PE	1-Undecanol	C11H24O	112-42-5	53.40	1.45
SAMPLE 4	p-Benzoquinone, 2,6-di-tert-butyl-	C 14H20O2	719-22-2	69.11	1.88
S	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	64.81	1.76
	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	C17H24O3	82304-66-3	4.82	0.13
	Dipropylene glycol	C6H14O3	110-98-5	5.43	0.15
	2-Propanol, 1,1'oxybis-	C6H14O3	110-98-5	8833.31	240.27
SAMPLE 5	Dipropylene glycol	C6H14O3	110-98-5	5489.31	149.31
	Dipropylene glycol	C6H14O3	110-98-5	6351.70	172.77
	Ethanol, 2-(dodecyloxy)	C14H30O2	4536-30-5	63.86	1.74
	Diisobutyl phthalate	C16H22O4	84-69-5	1.92	0.05
	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	9.82	0.27
	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	13.26	0.36

Migration levels continued

	Name	Formula	CAS	Output	Potential	
				μg/kg	Migration	
				PET	ug/Kg in food	
9	2-Butenal	C ₄ H ₆ O	123-73-9	5155.20	140.22	
SAMPLE 6						
Ĭ	Nonanal	C ₉ H ₁₈ O	124-19-6	1145.84	31.17	
<i>\</i> S						
	Dodecanal	C12H24O	112-54-9	101.51	2.76	
	Dipropylene glycol	C6H14O3	110-98-5	770.38	20.95	
SAMPLE 7	Dipropylene glycol	C6H14O3	110-98-5	291.53	7.93	
₽	Dipropylene glycol	C6H14O3	110-98-5	366.56	9.97	
SAI	Linalool	C10H18O	78-70-6	20.72	0.56	
	α-Terpineol	C10H18O	98-55-5	37.32	1.02	
	Benzenesulfonamide N-butyl-	C10H15NO2S	3622-84-2	1.00	0.03	
	Benzyl alcohol	C ₇ H ₈ O	100-51-6	7.14	0.19	
	Nonanal	C9H18O	124-19-6	116.08	3.16	
	Decanal	C10H20O	112-31-2	78.40	2.13	
8 4	Ethanol, phenoxy-	C8H10O2	122-99-6	24.60	0.67	
SAMPLE 8	Biphenyl	C12H10	92-52-4	4.03	0.11	
SAI	Diphenyl ether	C12H10O	101-84-8	8.13	0.22	
	2,4-Di-ertbutylphenol	C14H22O	96-76-4	13.32	0.36	
	Isopropyl myristate	C17H34O2	110-27-0	53.54	1.46	
6	Negeral	COLI180	124 10 6	71 10	1.04	
SAMPLE 9	Nonanal	C9H18O	124-19-6	71.19	1.94	
Ĕ	1-Undecanol	C11H24O	112-42-5	129.59	3.52	
SA	Dodecanal	C12H24O	112-54-9	83.17	2.26	
	2-Butenal, (Z)-	C ₄ H ₆ O	15798-64-8	1033.58	28.11	
	2,4-Hexadiene, 2,5dimethyl-	C8H14	764-13-6	671.97	18.28	
o.	2,4-Hexadiene, 3,4dimethyl-,	C8H14	2417-88-1	789.95	21.49	
Н	Dipropylene glycol	C6H14O3	110-98-5	4765.67	129.63	
SAMPLE 10	Dipropylene glycol	C6H14O3	110-98-5	3062.13	83.29	
SAN	Dipropylene glycol	C6H14O3	110-98-5	3609.89	98.19	
,	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	C17H24O3	82304-66-3	18.55	0.50	
	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	7.94	0.22	

g) Description of the applied sampling strategy

Samples of input batches and their resultant output batches were collected. Samples were analysed for the following substances:

- Volatile substances,
- Semi-volatile substances,
- Non-volatile substances,
- Inorganic substances,
- Primary aromatic amines.

The analysis was carried out by an independent third-party analytical laboratory.

The Laboratory was chosen based on its experience and expertise in analysing PET samples and its relevant analytical equipment and validated methods.

h) Description of the analytical procedures and methods used.

Samples of PET input batches and corresponding output batches were labelled for traceability purposes and shipped in clear and hermetically sealed containers.

The analytical procedures and method used for the analysis of the samples as well as their limits of detection and quantification are summarised in Table 2.

Table 1. Applied analytical procedures and methods including their limits of detection and quantification.

	Analytical method	Sample Preparation	LOD	LOQ
Untargeted screening of volatile	HS-SPME-GC-MS			
substances	3min@80°C ^a			
Untargeted screening of semi-	HS-SPME-GC-MS	Dissolution with HFIP		
volatile substances	3min@80°C ^a	2.000.00.0		
untargeted screening of non-	UPLC-MS-QTOF pos +	Dissolution with HFIP		
volatile substances	neg mode ^c			
Targeted analysis of primary	UPLC-MS-MS ^d	Extraction with 3%		See
aromatic amines	01 20 1110 1110	acetic acid		table
Targeted analysis of inorganic	ICP-MS ^e			See
substances (Annex II of EU		Pressure digestion		table
10/2011)				

GC: Gas chromatography; MS: Mass spectroscopy; QToF: Quadrupole- time-of-flight; FID: Flame Ionisation Detector; LC: liquid chromatography; UPLC: *ultrahigh performance LC*; ICP: Inductively Coupled Plasma

Analysis of organic substances is done through a non-targeted screening of volatile, semi-volatile and non-volatile substances with different methods (Table 2).

For volatile substances, a solid phase microextraction in headspace mode connected to GC-MS method (HS-SPME-GC-MS) is used which is a versatile technique employed in a wide range of industries and research areas to identify, quantify, and characterize volatile and semi-volatile compounds in plastic/polymer samples. The concentration of the volatile and semi volatile compounds on the SPME microfibre increases a lot the sensitivity of the method in such a way that a few ppbs (1-50 depends on the compound) can be detected for most of the volatile substances. The adsorption conditions for SPME of 3 mins@80°C specifically allow the exhaustive extraction of volatile substances present in PET without degrading the sample. The detection is done by MS and the mass spectra were compared with a mass spectra library (NIST or WYLEY).

For semi-volatile and non-volatile substance, the samples were first extracted. The solvent and extraction conditions have been chosen to swell the polymer, without generating new substances (Nerin *et al.*, 2022). The extracts were analysed using GC/MS and LC/MS-QToF for semi-volatile and non-volatile substances, respectively. High-resolution MS detectors like the QToF provide accurate masses isotopic patterns and intensities, which can lead to theoretical information about composition of fragments (Peters *et al.* 2019). This allows for the identification of unknown NIAS.

The application ranges of the above used non-targeted screening methods overlap but the sensitivity of the methods is different. In case the same substance was detected by different methods, the highest concentration of both analyses was reported in paragraph 4.

For the screening for primary aromatic amines a dedicated method was used as the concentration level of interest is so low that general non-target screening methods cannot detect them (Nerin et al., 2022).

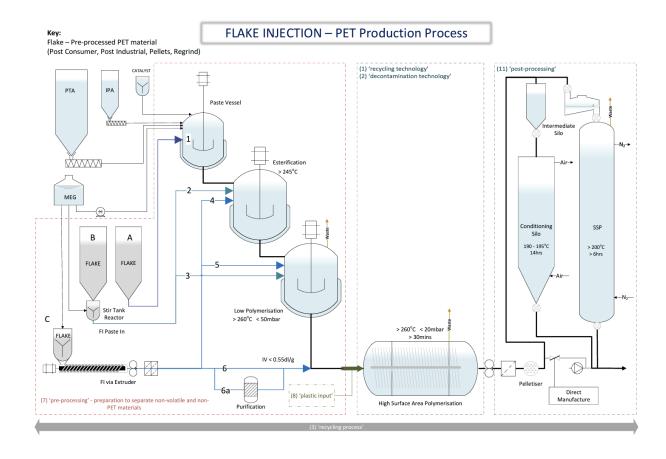
Inorganic substances were analysed using ICP-MS which is a sensitive elemental analysis technique that detects trace metals and non-metals at ultralow concentrations.

The Independent third-party laboratory follows ISO17025 quality control measures and all analytical methods are validated.

i) Analysis and explanation of any discrepancies observed between contaminant levels expected and decontamination efficiency.

No discrepancies have been observed between contaminant levels expected.

Appendix I –.



Glossary of Terms

Cmod Modelled concentration

DEG diethylene glycol

EG ethylene glycol

GC gas chromatography

HPLC high performance liquid chromatography

ICP-MS Inductively Coupled Plasma Mass Spectrometry

ICP-AES Inductively Coupled Plasma Atomic Emission Spectroscopy

IPA isophthalic acid

MHET mono(2-hydroxyethyl)terephthalate

MS Mass Spectrometry

NIAS non-intentionally added substances

PE polyethylene

PET polyethylene terephthalate

PP polypropylene

PVC polyvinyl chloride

TPA terephthalic acid

TTC Threshold of Toxicological Concern

XRF X-ray fluorescence spectroscopy

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