# PET materials and articles in which the recycled plastic is used behind a

# **Functional Barrier**.

## 3rd Monitoring Report

Monitoring Report by Article 13 of Regulation (EU) 2022/1616. 10th of October 2024.

Updated on October 16th. Text correction

## Contents

## Introduction

The novel technology for PET Functional barrier was notified as required under Article 10(2) and 10(3) of Commission Regulation (EU) 2022/1616 on 15th September 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.

This report should be read in conjunction with the Novel Technology notification dossier referred as "PET materials and articles in which the recycled plastics is used behind a Functional Barrier", submitted on 5 April 2023.

It is important to note that the safety and integrity of these materials is usually determined by extraction and/or migration and not by direct analysis of the polymer. The latter, although required by Regulation 2022/1616, is known to pose numerous technical problems in terms of obtaining reliable and reproducible results, it can generate substances that cannot be distinguished from contaminants and has therefore not been commonly used and has not been subjected to proficiency testing as reported in the scientific literature (Nerin et al., 2022)[1]

The results presented in this report are subject to further investigation for accuracy due to the large inter-laboratory and inter-sample variation observed. Significant sample degradation during analysis cannot be excluded at this time.

*The data presented in this report are based on the measurements performed by third-party laboratories, which were contracted by the members of the Functional Barrier (FB) Consortium formed by PETCORE-EUROPE and EuPC.. The data provided is the property of the FB consortium and cannot be copied, reproduced, or distributed without their prior written consent. The FB consortium is not responsible nor liable for any errors or inaccuracies that may have occurred during the measurement process by the third-party laboratories. The data are provided for informational purposes only and do not constitute any endorsement or recommendation by FB Consortium.*

[1] (PDF) Guidance in selecting analytical techniques for identification and quantification of non-intentionally added substances (NIAS) in food contact materials (FCMS) (researchgate.net)

## Forewords

The present document constitutes the report of the 3rd monitoring period for the Novel Recycling Technology "PET materials and articles in which the recycled plastic is used behind a Functional Barrier" for which a notification has been filed on April 5, 2023.

The present document is delivered in order to fulfil the requirements of Article 13: "Monitoring and reporting of contamination level".

In addition of the original notification dossier and the subsequent 1st and 2nd monitoring reports, the present monitoring report contains, among others,

1. An updated calculation of the potential migration of surrogate contaminants, replacing those reported in the paragraph entitled "Calculation of migration through a Functional Barrier", of the original notification dossier, carried out with the use of the commercial migration modelling software AKTS 365SML, Version 6.7 (AKTS- Sierre, Switzerland);
2. An updated list of the first 20 most occurring substances in the input materials, along with the decontamination efficiency calculated for selected representative substances;
3. The calculated specific migration in simulant D2 (95% ethanol) at time/temperature conditions of 10 days at 20°C, 10 days at 40°C and at 365 days 25°C, for three of the above mentioned most occurring substances, and two substances considered representative of the contamination, calculated with the above mentioned migration modelling software. The selected substances are: benzene (CAS N 71-43-2), limonene (CAS N 138-86-3), 2,2-Bis(4-hydroxyphenyl)propane (aka BPA) (CAS N 80-05-7), Terephthalic acid bis(2-ethylhexyl) ester (CAS N 6422-86-2), and Phthalic acid bis(2-ethylhexyl) ester (CAS N 117-81-7). Benzene and BPA were chosen as substances with high hazard profile, limonene represents a common contaminant from food, while, Terephthalic acid bis(2-ethylhexyl) ester and Phthalic acid bis(2-ethylhexyl) ester are indicators of contamination from plastics other than PET (e.g. PVC)
4. The actual specific migration of the above mentioned five substances in simulant D2 (95% ethanol), from sheets containing 100% RPET in the B layer and having A/B/A ratio of 7.5%/85%/7.5%, at time/temperature conditions of 10 days at 20°C, 10 days at 40°C and 10 days at 60°C

The paragraphs below contain the information required by Article13(5) of Regulation (EU) 2022/1616, covering the period from 10th April 2024 to 10th October 2024.

## Description of the Novel Recycling Technology- Art. 13(5)(a)

No modifications occurred in the Novel Recycling Technology, as it was described in the original notification dossier.

The Novel Recycling Technology, consists in the use of recycled PET (RPET) as central layer of structures A/B/A, where layer B is composed by RPET or blends of RPET with virgin PET, and layers A consist of virgin PET.

The manufacturing of A/B/A structures include a combination of some of the following processes:

- A drying and crystallization phase of the washed flakes, which is operated usually under stirring and air flow, at temperature of 140-160°C, generated by friction or IR, for a residence time up to 6 hours.
- An extrusion phase, where flakes are melted to produce the rPET B layer with or without application of vacuum. The temperature profile is usually 270-290°C. When vacuum is applied, the vacuum conditions are typically below 100 mbar.
- The coextrusion step, in which the A layers are applied in a die[2]. In this case the rPET of the future B layer comes in contact with the virgin PET (or mixture between virgin and mechanically recycled PET originated from a process that was object of a positive opinion delivered by EFSA) of the future A layers, at a temperature of typically 275-290°C. A 3-layer sheet (A/B/A) comes out from the coextrusion process and it is cooled down in a rolled stack press.
- The final thermoforming phase, in which the sheet is converted into trays. The sheet is heated in an oven to a temperature of 120-130°C, and the tray is formed through the application of pressure and vacuum in a mould. The total cycle takes 2-3 seconds. The tray is then immediately cooled down to an average temperature of around 30°C.

The following configurations (reported in Table 1) of processes are covered by the Novel Technology dossier:

Table 1: configurations of the equipment covered by the notification.

| Configurations | Crystallizing/drying | **Extrusion** | **Degassing** |
|---|---|---|---|
| X1 | yes | Single Screw | No |
| X2 | yes | Single Screw | Yes |
| Y1 | yes | Twin Screw Co-Rotating | Yes |
| Y2 | no | Twin Screw Co-Rotating | Yes |
| W | no | Single screw and satellitar | Yes |

In all the processes operating the equipment reported in Table 1, washed and dried RPET flakes are supplied to converters, accompanied by suitable specifications, and are co-extruded to produce the A/B/A structures with different A/B/A ratio and different thickness.

In case more information on the process is needed we suggest consulting the original notification dossier at https://www.petcore-europe.org/functional-barrier.html

## Capability of the process to produce safe materials - Art. 13(5)(b)

In the original notification dossier the data of decontamination capability calculated from challenge tests carried out in actual processes representing the equipment configurations of Table 1, were used to determine the maximum concentration of RPET in the B layer at which the safe level of migration of surrogates is met.

[2] Kostic, Milivoje & Reifschneider, Louis. (2006). Design of Extrusion Dies. Encyclopaedia of Chemical Processing. (PDF) Design of Extrusion Dies (researchgate.net)

The above mentioned commercially available migration simulation software AKTS365SML Version 6.7 was used for that purpose. In this 3rd report we have updated that calculation by operating the following improvements:

1. The number of structures on which the migration simulation was made increased from 3 to 5 (adding the total thickness of 120 micron and 700 micron)
2. The A/B/A ratio of 7.5/85/7.5 was added
3. The percentage of 30% of RPET in the B layer was added
4. The density of PET in the melt during the migration simulation was set at 1.2 g/cm3 (instead of 1.4 g/cm3 as in the original notification dossier). This was done because the density of Polyethylene Terephthalate (PET) in its melt state at 280°C typically ranges from 1.15 to 1.35 g/cm³**.** At elevated temperatures, like 280°C, PET's density decreases compared to its solid-state density due to the increased molecular mobility and expansion in the melt phase [3]
5. The density of PET in the solid phase during the migration simulation was set at 1.375 g/cm3 (instead of 1.4 g/cm3 as in the original notification dossier). This value is in line with the most updated parameters suggested by EFSA while conducting migration simulation calculations[4]
6. The parameters and conditions chosen for the migration simulation are summarized in Table 2. In this Table, the "realistic" conditions correspond to the choice in the migration software of an equation ("Piringer realistic equation") that does not include overestimation factors. This choice was made to avoid excessive and unrealistic overestimation of the diffusion of surrogate contaminants during the contact of recycled and virgin polymers in the melt phase. On the contrary, the "upper bound" conditions used in Step 5 correspond to the use of an equation that includes overestimation[3]. The thickness used in the migration simulation was divided by 2.5 in the step of thermoforming, considering the draw ratio as reported in the plot of Figure 2A of the original notification[5].

Table 2: conditions under which the simulation of migrations were simulated

| | | temperature(°C) | time | contact with food | Density | Tau | Ap' | equation | thickness |
|---|---|---|---|---|---|---|---|---|---|
| Step 1 | EXTRUSION | 280 | 0.33 min | NO | 1.2 | 1577 | 3.2 | realistic PET > 70°C | total |
| Step 2 | STORAGE | 25 | 180 days | NO | 1.375 | 1577 | -1.5 | realistic PET <70°C | total |
| Step 3 | THERMOFORMING | 125 | 10 sec | NO | 1.375 | 1577 | 3.2 | realistic PET > 70°C | total /2.5 |
| | | | | | | | | | |
| Step 4 | STORAGE | 25 | 180 days | NO | 1.375 | 1577 | -1.5 | realistic PET <70°C | total/2.5 |
| | | | | | | | | | |
| Step 5 | CONTACT WITH FOOD | 25 | 365 days | YES | 1.375 | 1577 | 3.1 | upper bound PET <70°C | total/2.5 |
| | | 40 | 10 days | | | | | | |
| | | 20 | 10 days | | | | | | |

[3] Brandrup, J., Immergut, E. H., & Grulke, E. A. (1999). "Polymer Handbook" (4th Edition). Wiley-Interscience

[4] EFSA Scientific Guidance on the criteria for the evaluation and on the preparation of applications for the safety assessment of post-consumer mechanical PET recycling processes intended to be used for manufacture of materials and articles in contact with food; DOI: 10.2903/j.efsa.2024.8879, 11.06.2024

[5] Reference is made to Figures 2a and 2b of the original notification (p. 6), which show examples of the most common distribution of draw ratios applied to produce thermoforms for protein and bakery products, and for fruits and vegetables, respectively

Calculations have been made executing Step 1 to Step 5. Then another calculation has been made using only step 1 and 5 (omitting steps 2 to 4). The outcomes of the simulation carried out by using Step 1 immediately followed by Step 5 do not differ from that the outcomes of the simulation with all the steps 1 to 5. Two examples of such an equivalence are provided in Annex I.

The equivalence between both methods suggests that the omission of Steps 2 to 4 do not significantly impact the migration calculation, which may imply these steps are not critical for the specific contaminants or materials under study. This also implies that modifications of the storage conditions, e.g. extending to 365 days instead of 180 days, would have a negligible impact on the final outcomes.

We have therefore decided to calculate the simulated migration by using Step 1 plus Step 5 instead of simulating all steps.

The charts provided in Annex II show the results of the simulated migration as a function of the total thickness of the sheets for different A/B/A structures, different percentage of RPET and different packaging conditions. The curves represented in the charts also contain the 2$^{nd}$ grade polynomial equation that can be used for the interpolation and extrapolation to different thickness' values.

The data presented in the charts have been calculated from an initial concentration of surrogates, designed as the "worst-case" scenario of 300 ppm of surrogate. This initial concentration is different from the 3 ppm used by EFSA, consequently the limit becomes 15 ppb instead of 0.15 ppb used by EFSA.

The points illustrated in the charts corresponds to the simulated migration of the surrogate contaminants showing highest value.

For the technology Y1Y2 this surrogate corresponds to Benzophenone at all simulated time/temperature conditions and for all thickness values.

For the technology X1X2W this surrogate corresponds to Benzophenone at all simulated time/temperature conditions for thickness values less or equal than 700 micron and becomes Chloroform at all simulated time/temperature conditions for thickness values higher than 700 microns.

## Most occurring substances - Art. 13(5)(c)

The analysis of substances with a molecular weight of up to 1000 Dalton has been made by screening methods performed by 9 different laboratories. The number of samples has been extended from the previous monitoring report. More than 160 samples for input and the correspondent 160 samples for output sheet after decontamination have been performed. The screening of the above mentioned monitoring has resulted in the development of two lists presented in Annex III, for the input material and Annex IVa and IVb for the output materials (respectively for technologies X1X2W and Y1Y2. These annexes provide an overview of the substances detected and categorized during the screening process, respectively for the incoming material and for the output, as a function of the technology configuration. In these Annexes are reported all substances detected with a minimum frequency of 3%, substances occurring at a lower frequency have been considered adventitious contaminants and not reported in the tables. Furthermore, a newly updated list, detailing the 20 most frequently occurring substances in input materials, has been developed. This new list highlights the occurrences and variations of substances, allowing for a more in-depth understanding of their distribution.

The difference between the newly generated list of substances and the data presented in the second monitoring report can be attributed to a significantly larger set of samples tested. This expansion of sample size has provided a more comprehensive overview of the distribution of substances within the analysed materials.

By increasing the number of samples, the results become in principle more statistically representative of the input and the output materials. This comprehensive approach enables to make better assessments of substance occurrence and the behaviour during recycling processes. It also improves the ability to compare results between different reports, such as the second monitoring report and the current analysis.

Three distinct types of substances have been identified in the recycled PET material:

1. Substances that are often introduced into the input material due to the use of PET in food contact applications. Examples include substances such as limonene and acetophenone. These contaminants enter the material during its initial use phase and can persist to some extent through the recycling process.
2. PET-Related Substances: These are substances inherent to the chemical composition of PET or are generated during the recycling process. Examples include acetaldehyde and PET oligomers.
3. Substances originating from contaminating polymers: These substances are formed as byproducts when contaminating polymers are subjected to heat or other recycling conditions. For example, benzene is generated from residues of PVC, styrene from residues of polystyrene, BPA from residues of polycarbonate[3]

## Decontamination efficiency – Art. 13(5)(c)

The decontamination efficiency of the recycling technologies used was evaluated specifically for contaminants in the PET materials. This evaluation was carried out by comparing the concentration of contaminants in the input materials to their concentration in the output materials after undergoing decontamination processes.

One of the key challenges in assessing decontamination efficiency by NIAS analysis, method that is not comparable to a challenge test, lies in accurately correlating the variability and dispersion of input data with the corresponding variability and dispersion in output results. This inconsistency is largely due to differences in sample collection techniques and the variety of analytical methods used across laboratories. Each laboratory has adopted distinct procedures and conditions for measuring the concentration of substances, leading to a scattered range of results. Variations in analytical conditions can have a profound effect on the concentration readings of substances. Consequently, the data may exhibit significant scatter, which makes it difficult to determine clear patterns or trends in decontamination effectiveness across different technologies.

This dispersion of data emphasizes the need for standardized analytical methods. By aligning laboratory procedures and adopting a uniform approach to testing, the comparability of decontamination data can be improved. As previously outlined, misalignments of laboratory practices represented a liming factor in our analysis.

While the decontamination efficiency has been calculated for contaminants, it has not been computed for substances that are either naturally present in PET or generated during the recycling process. These polymer-related substances, such as acetaldehyde and PET oligomers are part of the intrinsic properties of PET or byproducts of the polymer's breakdown during processing.

Annex V provides a detailed list of the 20 most frequently occurring substances in the input materials, occurrence rates and variation between input and output.

## Contaminating materials in the plastic input - Art. 13(5)(d)

The contaminating materials present in the plastic input are controlled by the specifications delivered by the producers of flakes.

The content of food grade PET in the plastic input is ≥95%. Other contaminants include:

- PVC ≤ 50 ppm
- Polyolefins ≤ 100 ppm
- Other plastics ≤ 50 ppm
- Metals ≤ 10 ppm
- Paper and wood fibres ≤ 10 ppm
- Other inert materials ≤ 5%

## Origin of the identified contaminants- Art. 13(5)(e)

The potential origin of the identified contaminants is under development. It will be reported in the next monitoring period.

## Measure or estimation of migration - Art. 13(5)(f)

ABA sheets containing different percentage of virgin and RPET have been analysed in order to carry out a complete screening of intentional and non-intentionally added components. The analysis has been carried out on sheets submitted to cryogenic grinding, and subsequently extracted in conditions described under the paragraph "Sampling strategy and analytical method". This allowed to detect the concentration of all substances present in the sheets.

Five most representative substances have been selected, namely

1. Benzene, substance formed during the degradation of PVC present as a contaminant in the input material. It is not excluded, however that benzene may also be generated by certain analytical methods
2. 2,2-bis(4-hydroxyphenyl)propane (aka BPA), formed from contamination of the input material by polycarbonate and also contamination from other sources (e.g. inks, coatings etc.)
3. Limonene, substance present because of contamination by food (juices, soft drinks in PET bottles)
4. Terephthalic acid, bis(2-ethylhexyl) ester, substance used as plasticiser, to replace Phthalic acid, bis(2-ethylhexyl) ester. It is the result of a contamination by other polymers (e.g. PVC).
5. Phthalic acid, bis(2-ethylhexyl) ester while widely replaced is still used as plasticiser, and usually represents an indicator of contamination by PVC (most probably by labels).

For the five substances mentioned above the following analysis have been carried out

- Simulation of migration with the AKTS software,
    - From an hypothetical monolayer sheet of 300 micron, containing the five substances at the concentration measured experimentally in the ground sheets samples

containing 100% RPET in the B layer. This calculation does not consider the presence of a functional barrier

- From ABA structures with various ABA ratio and referring the measured concentration of the five substances to the B layer only (i.e. considering that they are present as contaminants in the original RPET). This implies a correction of the concentration of these substances accounting for the dilution introduced by the A layers. This calculation considers the presence of a functional barrier

The parameters for calculation of migration were: surface-to-volume ratio of 6 sq.dm/1000 ml, conditions 10 days at 20°C, 10 days at 40°C and 365 days at 25°C. The results are reported in Table 3.

- Experimental migration tests in D2 simulant (95% ethanol) carried out from two ABA sheets respectively of 300 (manufactured by the X1X2W technology configuration) and 340 micron thickness (manufactured by the Y1Y2 technology configuration), with ABA ratio of 7.5/85/7.5 and 100% of RPET in the B layer, at conditions 10 days at 20°C, 10 days at 40°C and 10 days at 60°C. The results are reported in Table 5, for the five substances respectively in Table 4.1, 4.2, 4.3, 4.4 and 4.5

The results of the simulation and of the actual migration are reported in Table 4. For a proper interpretation of Table 4, the following should be taken into account:

1. The data corresponding to “results_nonscaled_output” refers to concentration of the substances measured in the sheets, after grinding, with the method described in the paragraph "Sampling strategy and analytical method”;
2. The data corresponding to “results_scaled_output” refers to the same concentration, corrected as the substances were in B layer only (considering the dilution caused by layers A)
3. The results of simulation of migration (ppb)- data from "results_nonscaled_output" have been calculated from a sheet of mono-layer with 300 micron thickness, assuming that the concentration of the ground sample is equally distributed in the whole sheet
4. The results of simulation of migration (ppb)- data from “results_scaled_output” have been calculated for sheets of 300 micron thickness, with ABA ratio corresponding to the “ABA structures” column.

The results show that the simulation of migration carried out on sheets having the measured concentration in layer B are in line with the experimental measures, except for benzene.

This requires more investigation, that will be carried out during the next monitoring period.

The results also show that actual migration of the substances in the tested conditions is almost always “not detectable”, with the exception of benzene at 10 days/40°C and 10 days/60°C .

As expected, the analytical test does not have a sufficient LOD to detect the substances at the level calculated in the simulation of migration.

Table 3: results of migration simulation of the selected substances detected in the sheets

| substance | ABA structures | average conc of the substance in the sheet (results_nonscaled_output)/ (ppb) | average conc of the substance in the sheet (resultsscaled_output)/ (ppb) | results of simulation of migration (ppb)- data from "results_nonscaled_output" Thickness: 300 micron | | | results of simulation of migration (ppb)- data from "results_scaled_output" Thickness: 300 micron/ ABA structures | | |
|---|---|---|---|---|---|---|---|---|---|
| | | results referred only to sheets with 100% RPET in B layer | | 10 days 20°C | 10 days 40°C | 365 days 25°C | 10 days 20°C | 10 days 40°C | 365 days 25°C |
| benzene | **5/90/5** | 1594,00 | 1778,00 | 0,33 | 1,21 | 2,78 | <0.01 | 0,07 | 1,09 |
| | **7,5/85/7,5** | 960,00 | 1123,00 | 0,20 | 0,73 | 1,67 | <0.01 | 0,01 | 0,36 |
| | **10/80/10** | 1002,00 | 1250,00 | 0,21 | 0,76 | 1,75 | <0.01 | <0.01 | 0,19 |
| | **15/70/15** | 526,00 | 707,00 | 0,11 | 0,40 | 0,92 | <0.01 | <0.01 | 0,02 |
| limonene/d-limonene | **5/90/5** | 335,00 | 371,00 | 0,04 | 0,16 | 0,37 | <0.01 | <0.01 | 0,07 |
| | **7,5/85/7,5** | 136,00 | 160,00 | 0,02 | 0,06 | 0,15 | <0.01 | <0.01 | 0,01 |
| | **10/80/10** | 200,00 | 250,00 | 0,03 | 0,10 | 0,22 | <0.01 | <0.01 | <0.01 |
| | **15/70/15** | 112,00 | 155,00 | 0,01 | 0,05 | 0,12 | <0.01 | <0.01 | <0.01 |
| 2,2-bis(4-hydroxyphenyl)propane | **5/90/5** | 1779,00 | 1971,00 | 0,13 | 0,47 | 1,07 | <0.01 | <0.01 | <0.01 |
| | **7,5/85/7,5** | 1974,00 | 2308,00 | 0,14 | 0,52 | 1,19 | <0.01 | <0.01 | <0.01 |
| | **10/80/10** | 2296,00 | 2831,00 | 0,16 | 0,60 | 1,38 | <0.01 | <0.01 | <0.01 |
| | **15/70/15** | 1027,00 | 1375,00 | 0,07 | 0,27 | 0,62 | <0.01 | <0.01 | <0.01 |
| terephthalic acid, bis(2-ethylhexyl)ester | **5/90/5** | 265,51 | 296,64 | 0,01 | 0,03 | 0,07 | <0.01 | <0.01 | <0.01 |
| | **7,5/85/7,5** | 1851,00 | 2167,79 | 0,06 | 0,21 | 0,48 | <0.01 | <0.01 | <0.01 |
| | **10/80/10** | 2156,59 | 2695,74 | 0,07 | 0,24 | 0,56 | <0.01 | <0.01 | <0.01 |
| | **15/70/15** | 6740,00 | 8981,37 | 0,21 | 0,76 | 1,75 | <0.01 | <0.01 | <0.01 |
| phthalic acid, bis(2-ethylhexyl) ester | **5/90/5** | 567,00 | 656,00 | 0,02 | 0,06 | 0,15 | <0.01 | <0.01 | <0.01 |
| | **7,5/85/7,5** | 697,00 | 934,00 | 0,02 | 0,08 | 0,18 | <0.01 | <0.01 | <0.01 |
| | **10/80/10** | 446,00 | 557,00 | 0,01 | 0,05 | 0,12 | <0.01 | <0.01 | <0.01 |
| | **15/70/15** | 2087,00 | 3057,00 | 0,06 | 0,24 | 0,54 | <0.01 | <0.01 | <0.01 |

Table 4 – migration results of the selected substances detected in the sheets

Table 4.1 - migration results of Benzene

| Technology Configuration | LAB | CONDITIONS | Substance | Migration 1 ppb | Migration 2 ppb | Migration 3 ppb | Average migration ppb | LOD ppb | Simulation ABA- ppb |
|---|---|---|---|---|---|---|---|---|---|
| Y1 / Y2 | LAB a | 10d-20ºc | Benzene | ND | ND | ND | ND | 0.06 | <0.01 |
| | LAB b | | | ND | ND | ND | ND | 1.20 | |
| | LAB c | | | ND | ND | ND | ND | 1.50 | |
| | LAB d | | | ND | ND | ND | ND | 0.18 | |
| X1 / X2 / W | LAB a | | | ND | ND | ND | ND | 0.06 | |
| | LAB b | | | ND | ND | ND | ND | 1.20 | |
| | LAB c | | | ND | ND | ND | ND | 1.50 | |
| | LAB d | | | ND | ND | ND | ND | 0.18 | |
| Y1 / Y2 | LAB a | 10d-40ºc | | 2.0 | 2.0 | 2.0 | 2.0 | 0.06 | 0.01 |
| | LAB b | | | ND | ND | ND | ND | 1.20 | |
| | LAB c | | | ND | ND | ND | ND | 1.50 | |
| | LAB d | | | 0.8 | 0.8 | 0.8 | 0.8 | 0.18 | |
| X1 / X2 / W | LAB a | | | 0.3 | 0.3 | 0.4 | 0.3 | 0.06 | |
| | LAB b | | | ND | ND | ND | ND | 1.20 | |
| | LAB c | | | ND | ND | ND | ND | 1.50 | |
| | LAB d | | | ND | ND | ND | ND | 0.18 | |
| Y1 / Y2 | LAB a | 10d-60ºC | | 5.4 | 4.3 | 2.0 | 3.9 | 0.06 | |
| | LAB b | | | ND | ND | ND | ND | 1.20 | |
| | LAB c | | | ND | ND | ND | ND | 1.50 | |
| | LAB d | | | 11.4 | 11.4 | 10.8 | 11.2 | 0.18 | |
| X1 / X2 / W | LAB a | | | 1.9 | 1.9 | 1.9 | 1.9 | 0.06 | |
| | LAB b | | | ND | ND | ND | ND | 1.20 | |
| | LAB c | | | ND | ND | ND | ND | 1.50 | |
| | LAB d | | | 1.9 | 2.0 | 1.7 | 1.9 | 0.18 | |

Table 4.2 - migration results of limonene

| Technology Configuration | LAB | CONDITIONS | Substance | Migration 1 ppb | Migration 2 ppb | Migration 3 ppb | Average migration ppb | LOD ppb | Simulation ABA- ppb |
|---|---|---|---|---|---|---|---|---|---|
| X1 / X2 / W | LAB a | 10d-20ºc | **Limonene** | ND | ND | ND | ND | 6 | <0.01 |
| | LAB b | | | ND | ND | ND | ND | 1.2 | |
| | LAB c | | | ND | ND | ND | ND | 15 | |
| | LAB d | | | ND | ND | ND | ND | 0.6 | |
| Y1 / Y2 | LAB a | | | ND | ND | ND | ND | 6 | |
| | LAB b | | | ND | ND | ND | ND | 1.2 | |
| | LAB c | | | ND | ND | ND | ND | 15 | |
| | LAB d | | | ND | ND | ND | ND | 0.6 | |
| X1 / X2 / W | LAB a | 10d-40ºc | | ND | ND | ND | ND | 6 | <0.01 |
| | LAB b | | | ND | ND | ND | ND | 1.2 | |
| | LAB c | | | ND | ND | ND | ND | 15 | |
| | LAB d | | | ND | ND | ND | ND | 0.6 | |
| Y1 / Y2 | LAB a | | | ND | ND | ND | ND | 6 | |
| | LAB b | | | ND | ND | ND | ND | 1.2 | |
| | LAB c | | | ND | ND | ND | ND | 15 | |
| | LAB d | | | ND | ND | ND | ND | 0.6 | |
| X1 / X2 / W | LAB a | 10d-60ºC | | ND | ND | ND | ND | 6 | |
| | LAB b | | | ND | ND | ND | ND | 1.2 | |
| | LAB c | | | ND | ND | ND | ND | 15 | |
| | LAB d | | | ND | ND | ND | ND | 0.6 | |
| Y1 / Y2 | LAB a | | | ND | ND | ND | ND | 6 | |
| | LAB b | | | ND | ND | ND | ND | 1.2 | |
| | LAB c | | | ND | ND | ND | ND | 15 | |
| | LAB d | | | ND | ND | ND | ND | 0.6 | |

Table 4.3 - migration results of Bisphenol A

| Technology Configuration | LAB | CONDITIONS | Substance | Migration 1 ppb | Migration 2 ppb | Migration 3 ppb | Average migration ppb | LOD ppb | Simulation ABA-ppb |
|---|---|---|---|---|---|---|---|---|---|
| Y1 / Y2 | LAB a | 10d-20ºc | **Bisphenol A** | ND | ND | ND | ND | | <0.01 |
| | LAB b | | | ND | ND | ND | ND | 1.5 | |
| | LAB c | | | ND | ND | ND | ND | 6.0 | |
| | LAB d | | | ND | ND | ND | ND | | |
| X1 / X2 / W | LAB a | | | ND | ND | ND | ND | | |
| | LAB b | | | ND | ND | ND | ND | 1.5 | |
| | LAB c | | | ND | ND | ND | ND | 6.0 | |
| | LAB d | | | ND | ND | ND | ND | | |
| Y1 / Y2 | LAB a | 10d-40ºc | | ND | ND | ND | ND | | <0.01 |
| | LAB b | | | ND | ND | ND | ND | 1.5 | |
| | LAB c | | | ND | ND | ND | ND | 6.0 | |
| | LAB d | | | ND | ND | ND | ND | | |
| X1 / X2 / W | LAB a | | | ND | ND | ND | ND | 6.0 | |
| | LAB b | | | ND | ND | ND | ND | 1.5 | |
| | LAB c | | | ND | ND | ND | ND | 6.0 | |
| | LAB d | | | ND | ND | ND | ND | | |
| Y1 / Y2 | LAB a | 10d-60ºC | | ND | ND | ND | ND | | |
| | LAB b | | | ND | ND | ND | ND | 1.5 | |
| | LAB c | | | ND | ND | ND | ND | 6.0 | |
| | LAB d | | | ND | ND | ND | ND | | |
| X1 / X2 / W | LAB a | | | ND | ND | ND | ND | | |
| | LAB b | | | ND | ND | ND | ND | 1.5 | |
| | LAB c | | | ND | ND | ND | ND | 6.0 | |
| | LAB d | | | ND | ND | ND | ND | | |

Table 5.4 - migration results of Bis(2-ethylhexyl) terephthalate

| Technology Configuration | LAB | CONDITIONS | Substance | Migration 1 ppb | Migration 2 ppb | Migration 3 ppb | Average migration ppb | LOD ppb | Simulation ABA-ppb |
|---|---|---|---|---|---|---|---|---|---|
| **X1 / X2 / W** | LAB a | 10d-20ºc | **Bis(2-ethylhexyl) terephthalate** | ND | ND | ND | ND | 48.0 | <0.01 |
| | LAB b | | | ND | ND | ND | ND | 3.0 | |
| | LAB c | | | ND | ND | ND | ND | 60.0 | |
| | LAB d | | | ND | ND | ND | ND | 18.0 | |
| **Y1 /Y2** | LAB a | | | ND | ND | ND | ND | 48.0 | |
| | LAB b | | | ND | ND | ND | ND | 3.0 | |
| | LAB c | | | ND | ND | ND | ND | 60.0 | |
| | LAB d | | | ND | ND | ND | ND | 18.0 | |
| **X1 / X2 / W** | LAB a | 10d-40ºc | | ND | ND | ND | ND | 48.0 | <0.01 |
| | LAB b | | | ND | ND | ND | ND | 3.0 | |
| | LAB c | | | ND | ND | ND | ND | 60.0 | |
| **Y1 /Y2** | LAB a | | | ND | ND | ND | ND | 48.0 | |
| | LAB b | | | ND | ND | ND | ND | 3.0 | |
| | LAB c | | | ND | ND | ND | ND | 60.0 | |
| | LAB d | | | ND | ND | ND | ND | 18.0 | |
| **X1 / X2 / W** | LAB a | 10d-60ºC | | ND | ND | ND | ND | 48.0 | |
| | LAB b | | | ND | ND | ND | ND | 3.0 | |
| | LAB c | | | ND | ND | ND | ND | 60.0 | |
| | LAB d | | | ND | ND | ND | ND | 18.0 | |
| **Y1 /Y2** | LAB a | | | ND | ND | ND | ND | 48.0 | |
| | LAB b | | | ND | ND | ND | ND | 3.0 | |
| | LAB c | | | ND | ND | ND | ND | 60.0 | |
| | LAB d | | | ND | ND | ND | ND | 18.0 | |

Table 5.5 - migration results of Bis(2-ethylhexyl) phthalate

| Technology Configuration | LAB | CONDITIONS | Substance | Migration 1 ppb | Migration 2 ppb | Migration 3 ppb | Average migration ppb | LOD ppb | Simulation ABA-ppb |
|---|---|---|---|---|---|---|---|---|---|
| **X1 / X2 / W** | LAB a | 10d-20ºc | **Bis(2-ethylhexyl) phthalate** | ND | ND | ND | ND | 30.00 | <0.01 |
| | LAB b | | | ND | ND | ND | ND | 3.00 | |
| | LAB c | | | ND | ND | ND | ND | 60.00 | |
| | LAB d | | | ND | ND | ND | ND | 18.00 | |
| **Y1 / Y2** | LAB a | | | ND | ND | ND | ND | 30.00 | |
| | LAB b | | | ND | ND | ND | ND | 3.00 | |
| | LAB c | | | ND | ND | ND | ND | 60.00 | |
| | LAB d | | | ND | ND | ND | ND | 18.00 | |
| **X1 / X2 / W** | LAB a | 10d-40ºc | | ND | ND | ND | ND | 30.00 | <0.01 |
| | LAB b | | | ND | ND | ND | ND | 3.00 | |
| | LAB c | | | ND | ND | ND | ND | 60.00 | |
| | LAB d | | | ND | ND | ND | ND | 18.00 | |
| **Y1 / Y2** | LAB a | | | ND | ND | ND | ND | 30.00 | |
| | LAB b | | | ND | ND | ND | ND | 3.00 | |
| | LAB c | | | ND | ND | ND | ND | 60.00 | |
| | LAB d | | | ND | ND | ND | ND | 18.00 | |
| **X1 / X2 / W** | LAB a | 10d-60ºC | | ND | ND | ND | ND | 30.00 | |
| | LAB b | | | ND | ND | ND | ND | 3.00 | |
| | LAB c | | | ND | ND | ND | ND | 60.00 | |
| | LAB d | | | ND | ND | ND | ND | 18.00 | |
| **Y1 / Y2** | LAB a | | | ND | ND | ND | ND | 30.00 | |
| | LAB b | | | ND | ND | ND | ND | 3.00 | |
| | LAB c | | | ND | ND | ND | ND | 60.00 | |
| | LAB d | | | ND | ND | ND | ND | 18.00 | |

## Sampling strategy and analytical method - Art. 13(5)(g) and Art. 13(5)(h)

The tested samples have been provided by the consortium members, and were selected to represent commonly used flakes purchased in the market place and used by converters in the B layer, and ABA structures normally supplied to the market. All technologies were represented in the sampling. The samples were collected at regular intervals in the period from January to March 2024, and the tests were reported and elaborated in the 2nd Quarter of 2024.

The samples were tested by 9 laboratories located in different EU Countries, by using different test methods.

The screening analysis was carried out for

- Volatile substances
- Semi-volatile substances, and
- Non-volatile substances

The laboratories and relevant test methods are summarized in Annex V.

## Discrepancies between input and output - Art. 13(5)(i)

As previously outlined, some substances originate from the contamination of PET that occur in the use, disposal and collection phase. These substances are normally removed during the recycling process; for these substances a decontamination efficiency can be calculated as a percent difference between output and input material, and the resulting outcome will be a negative number (column z "difference_input_output" in the master sheet of Annex I.

On the contrary, some substances are generated during the processing; they only present in the output, or their quantity increases in the output compared to the input

## Discussion of differences from previous report- Art. 13(5)(j)

There are numerous differences introduced by this 3rd monitoring report compared with previous reports.

- An updated calculation of the potential migration of surrogate contaminants, replacing those reported in the paragraph entitled "Calculation of migration through a Functional Barrier", of the original notification dossier;
- An updated list of the first 20 most occurring substances in the input materials, along with the decontamination efficiency calculated for selected representative substances;
- The calculated specific migration in simulant D2 (95% ethanol) at time/temperature conditions of 10 days at 20°C, 10 days at 40°C and at 365 days 25°C, for five substances considered representative of the contamination
- The actual specific migration of the above mentioned five substances in simulant D2 (95% ethanol), from sheets containing 100% RPET in the B layer and having A/B/A ratio of

7.5%/85%/7.5%, at time/temperature conditions of 10 days at 20°C, 10 days at 40°C and 10 days at 60°C

# Annex I- Equivalence of simulation approaches

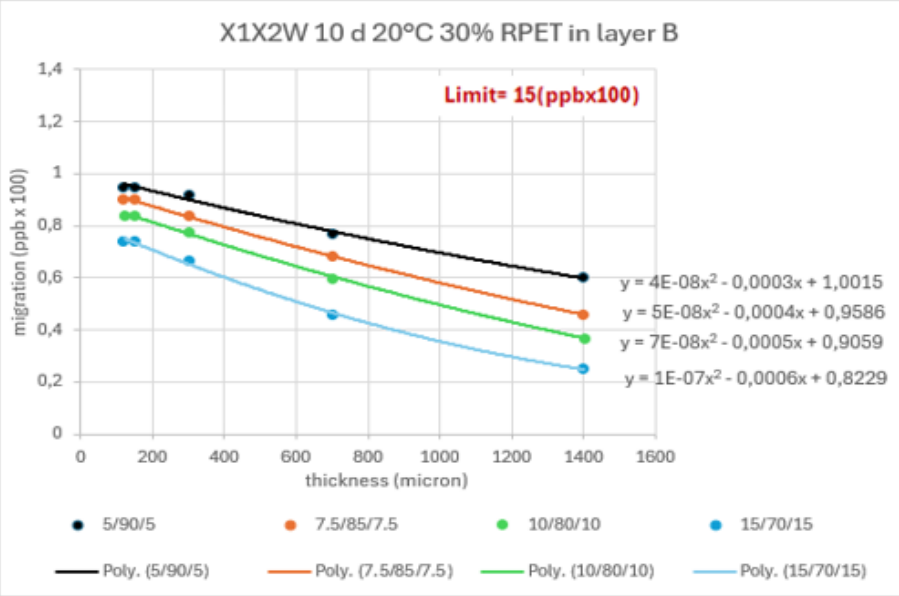
Annex I- Equivalence between simulation of migration made by calculating step 1,2,3 4 and 5 of Table 2, and by calculating steps 1 and 5 of the same Table

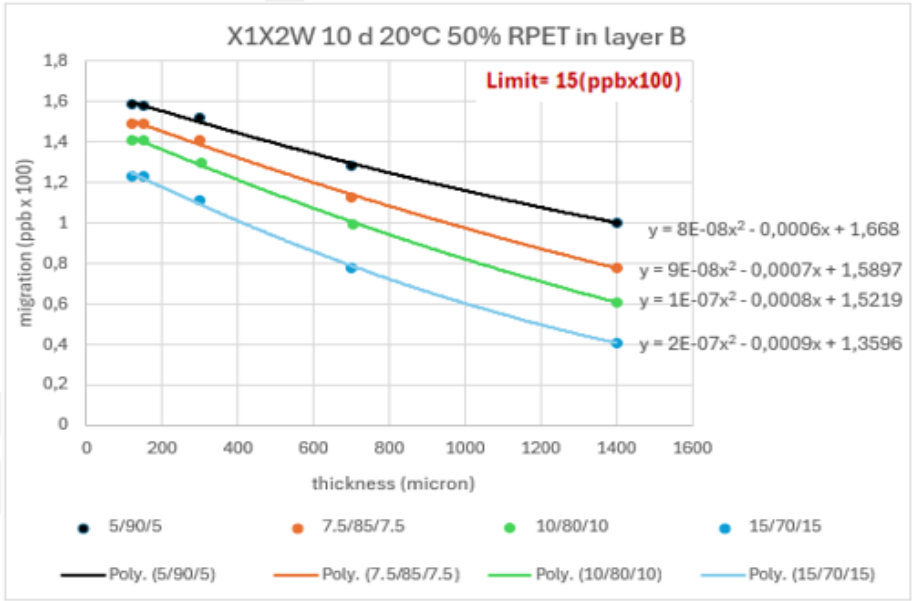
| y1-y2 | 365 d 25°C EtOH 95% | 50% R-PET |
|---|---|---|
| 300 my | Simplified calculations ppb | All Steps calculations ppb |
| ChloroBenzene | 12.19 | 12.20 |
| MethylSalicilate | 5.96 | 5.98 |
| Methyl Stearate | 13.32 | 13.50 |
| Phenylcyclohexane | 9.68 | 9.71 |
| Toluene | 11.92 | 11.92 |
| Benzophenone | 35.88 | 36.08 |
| Chloroform | 0 | 0 |
| thickness (5%-90%-5%) | 15-270-15 | 15-270-15 |

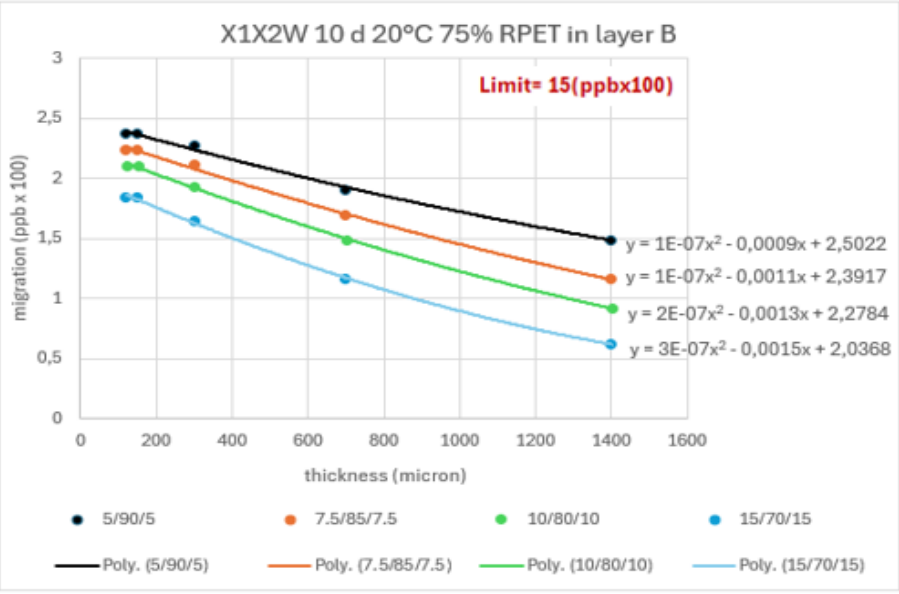
| X1-X2-W | 365 d 25°C EtOH 95% | 50% R-PET |
|---|---|---|
| 300 my | Simplified calculations ppb | All Steps calculations ppb |
| ChloroBenzene | 4.81 | 4.81 |
| MethylSalicilate | 8.04 | 8.06 |
| Methyl Stearate | 4.91 | 4.98 |
| Phenylcyclohexane | 6.83 | 6.86 |
| Toluene | 5.27 | 5.27 |
| Benzophenone | 13.00 | 13.07 |
| Chloroform | 12.22 | 12.23 |
| thickness (5%-90%-5%) | 15-270-15 | 15-270-15 |

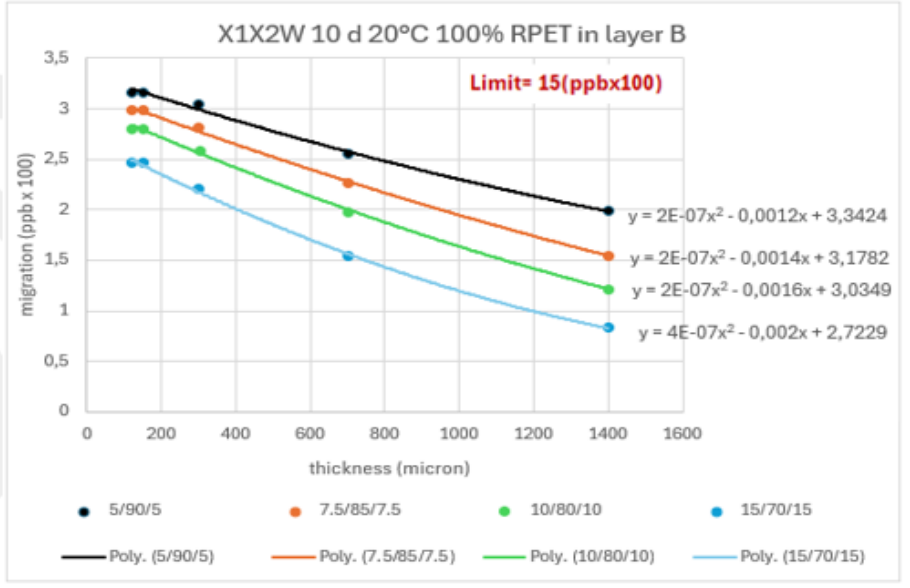
# Annex II- Simulated migration for different ABA structures

# X1X2W Configurations at 10 Days 20ºC

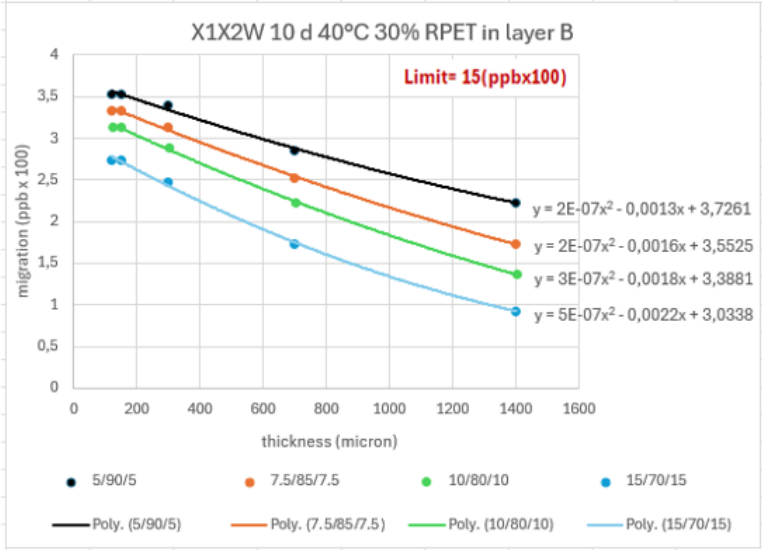


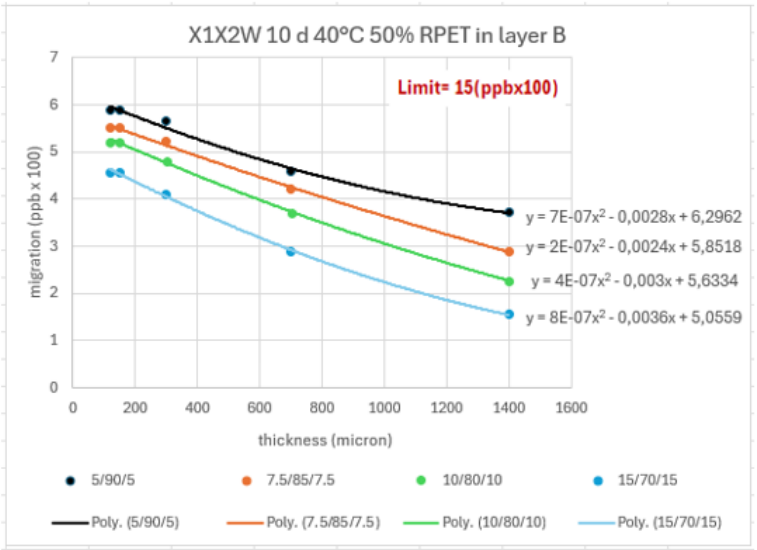



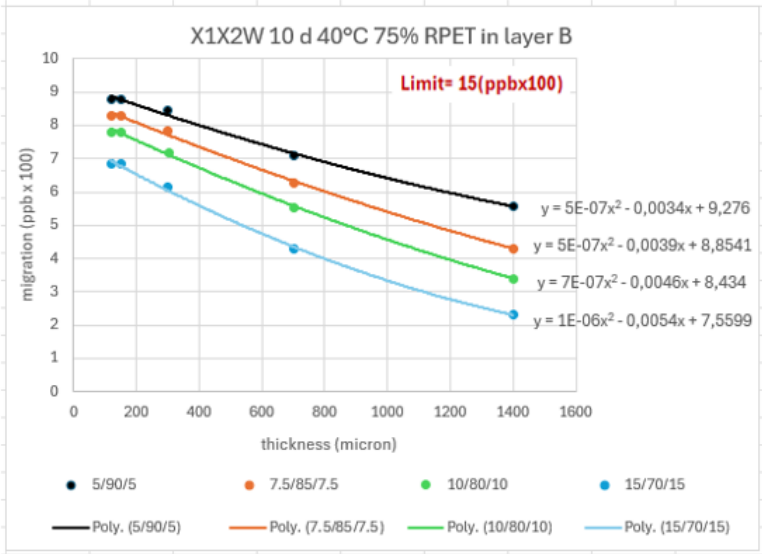



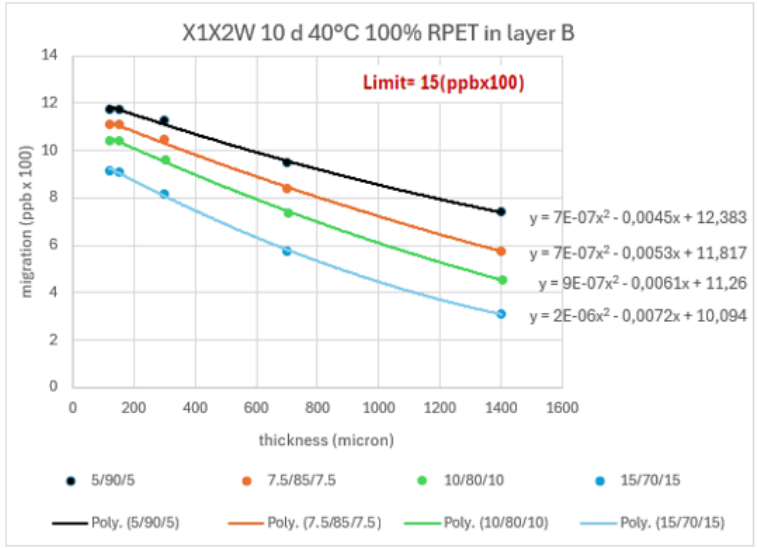



## X1X2W Configurations at 10 Days 40ºC

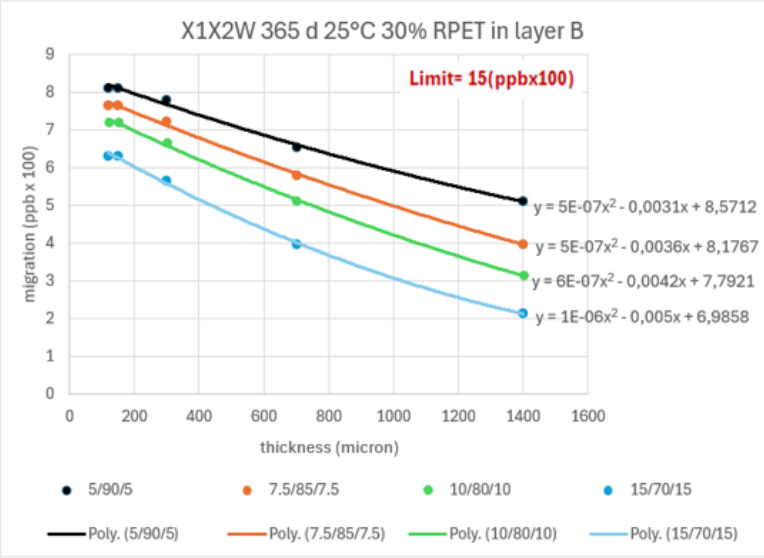


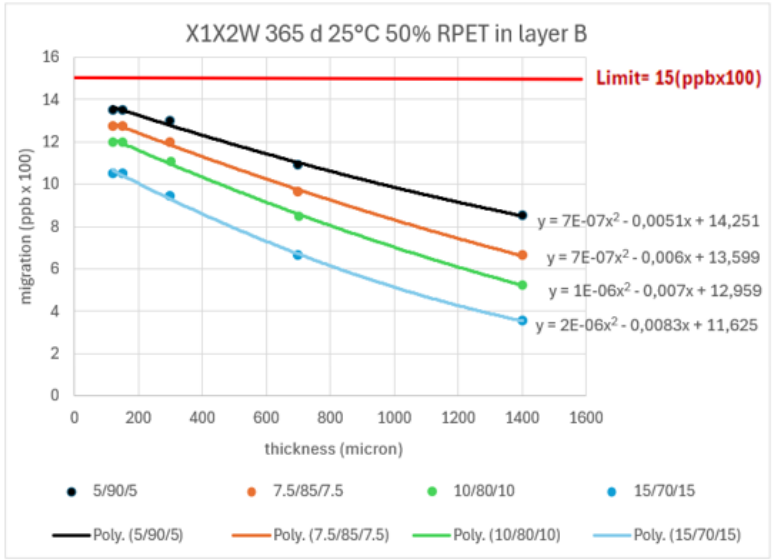



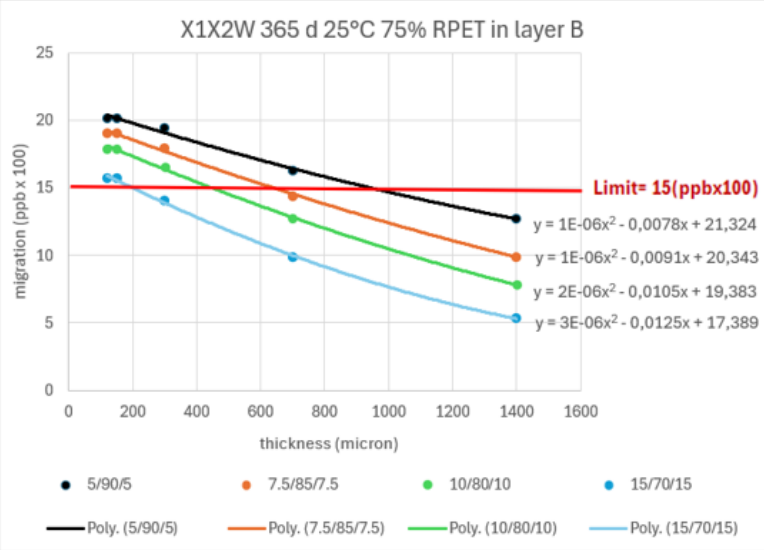



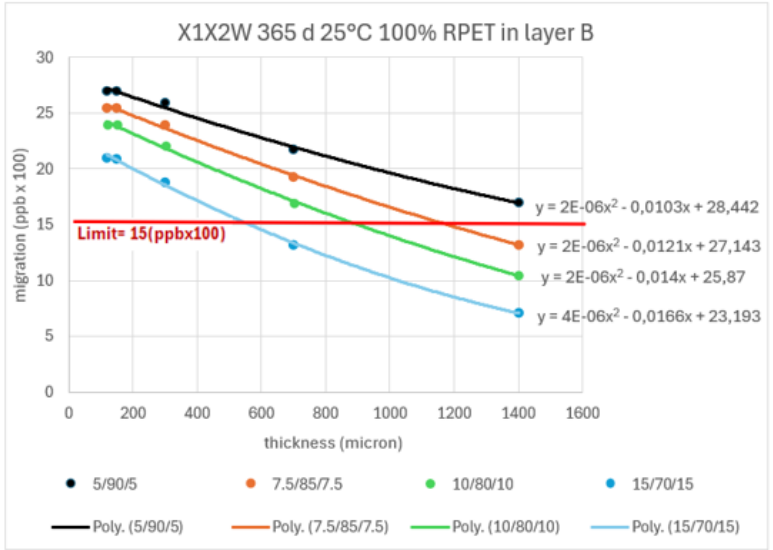



## X1X2W Configurations at 365 Days 25ºC

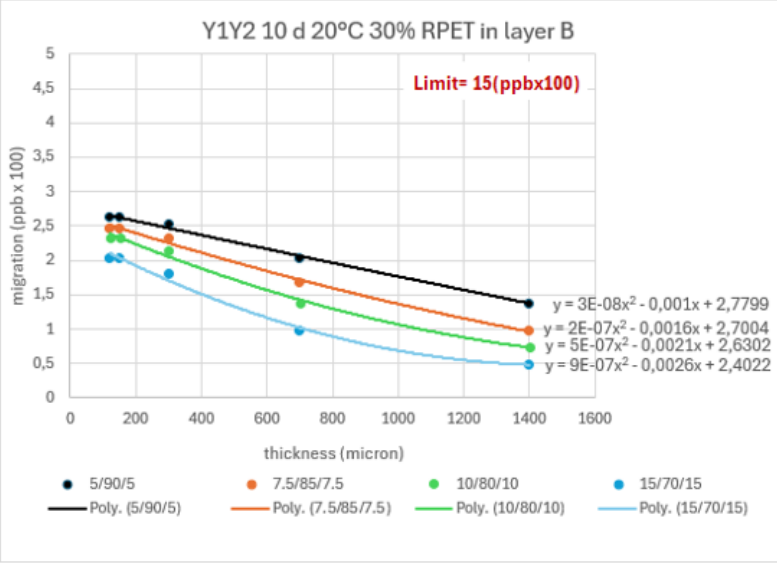


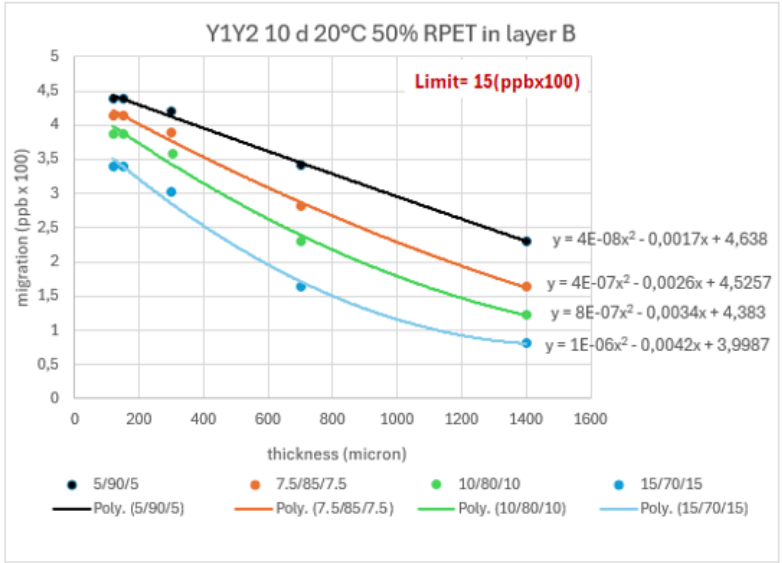



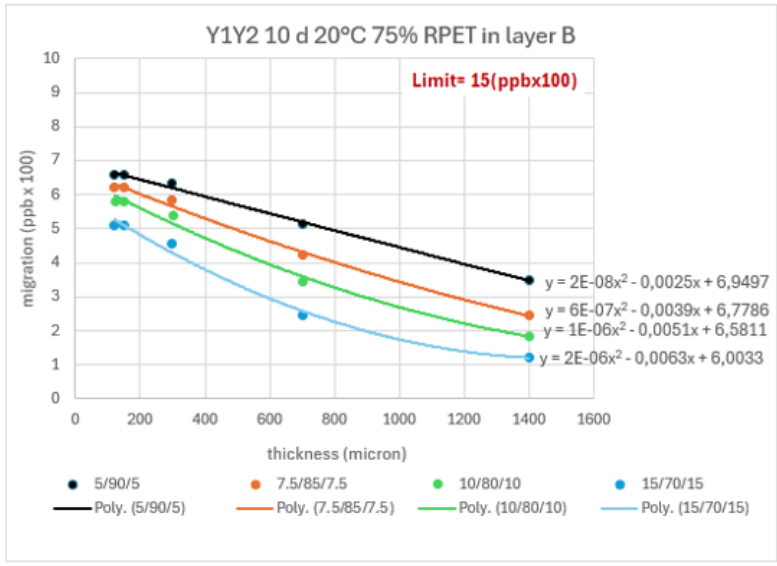



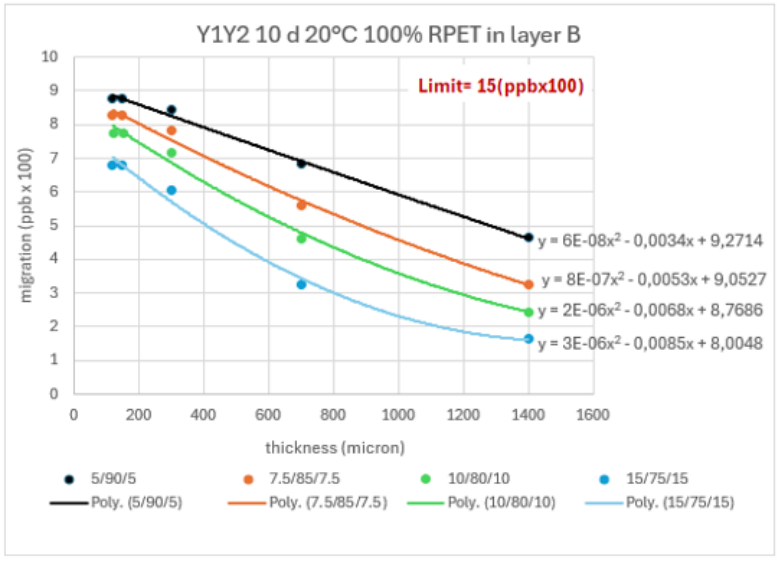



## Y1Y2 Configurations at 10 Days 20ºC

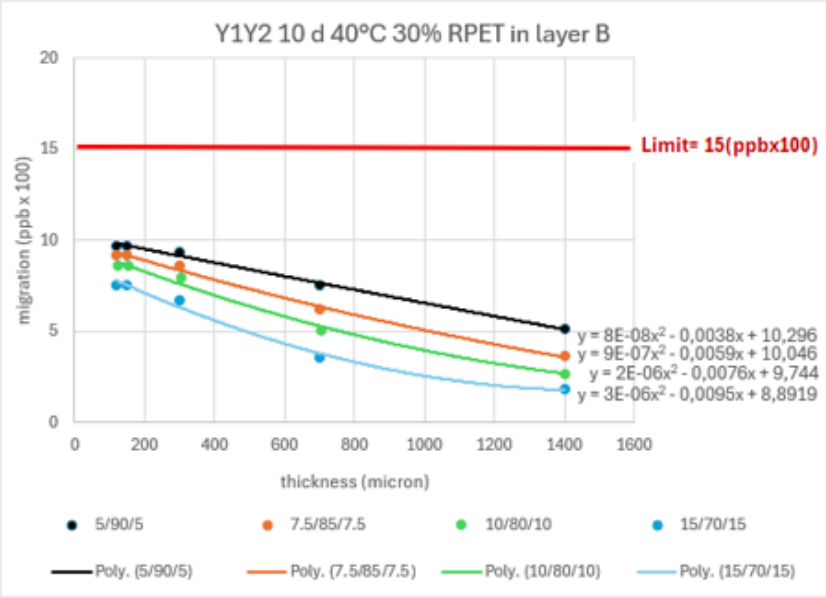


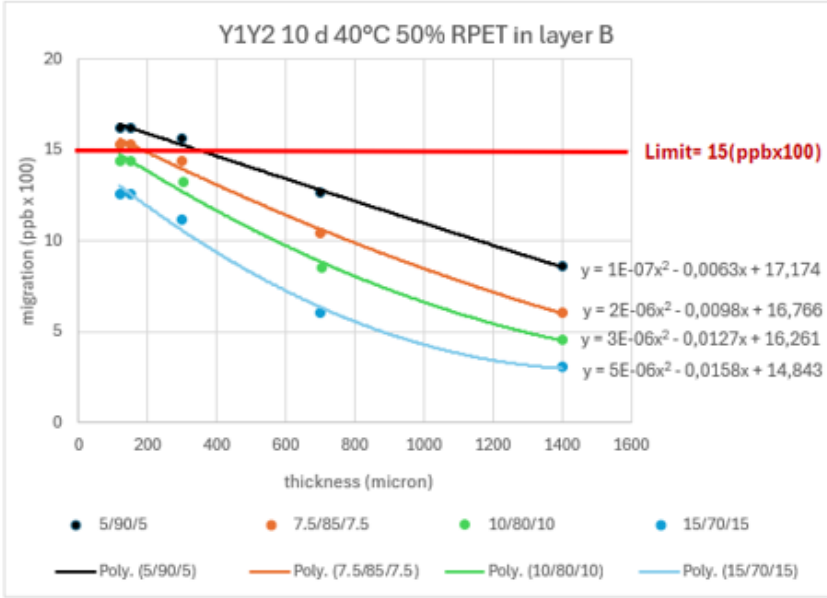



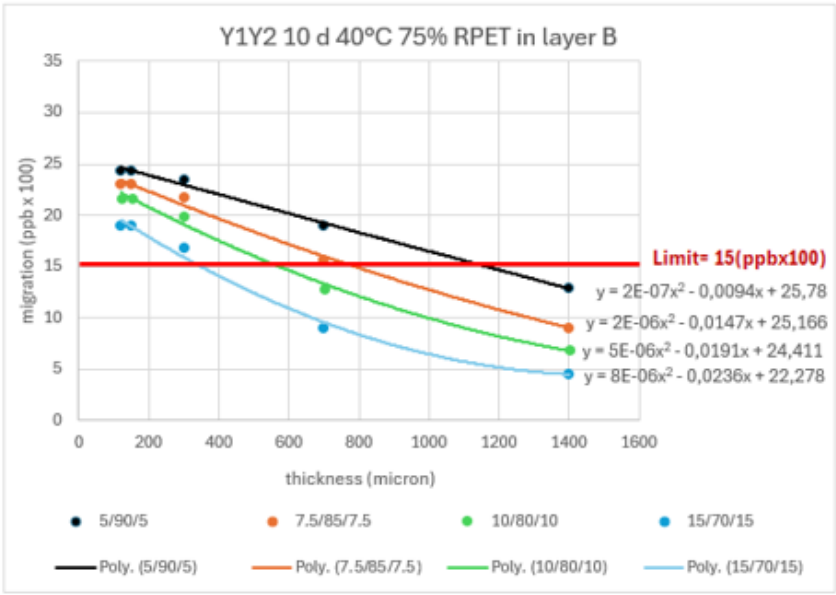



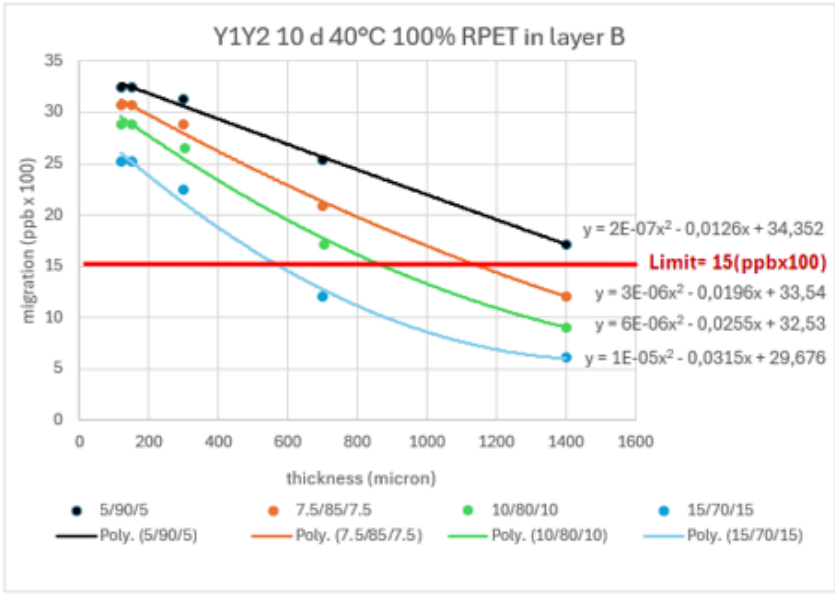



# Y1Y2 Configurations at 10 Days 40°C

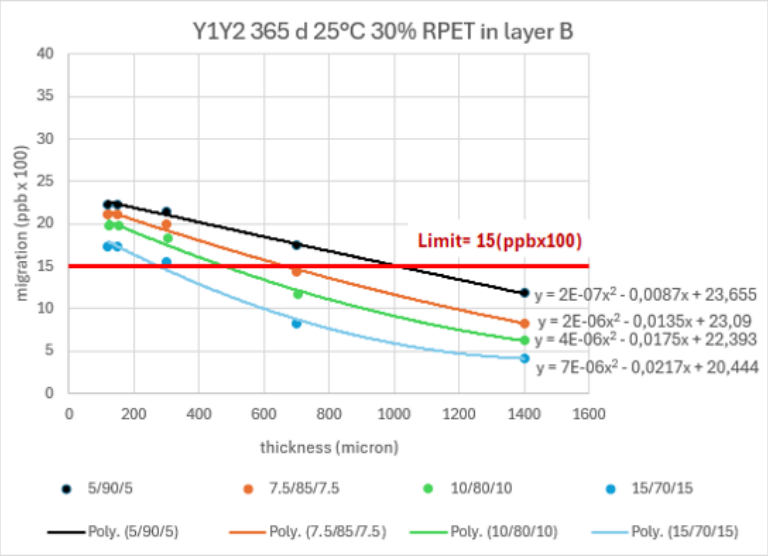


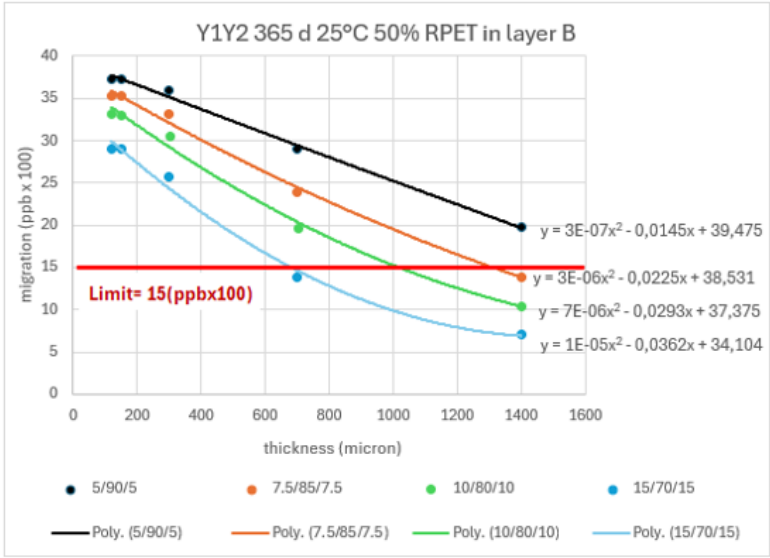



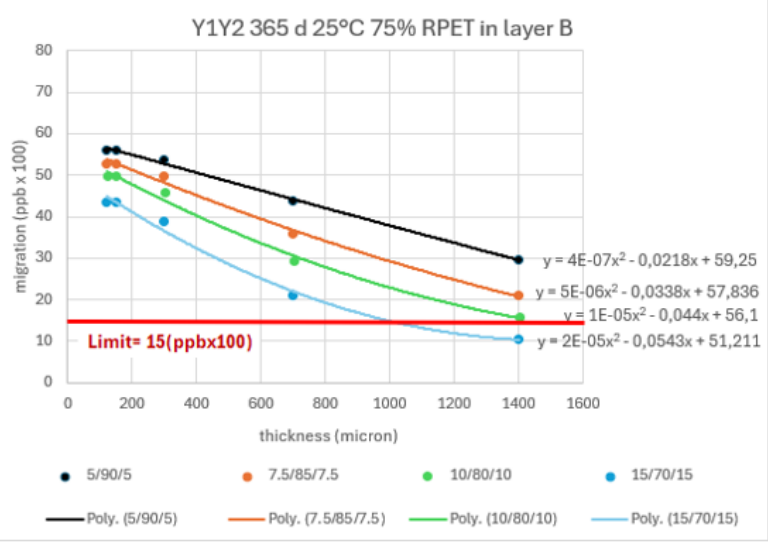



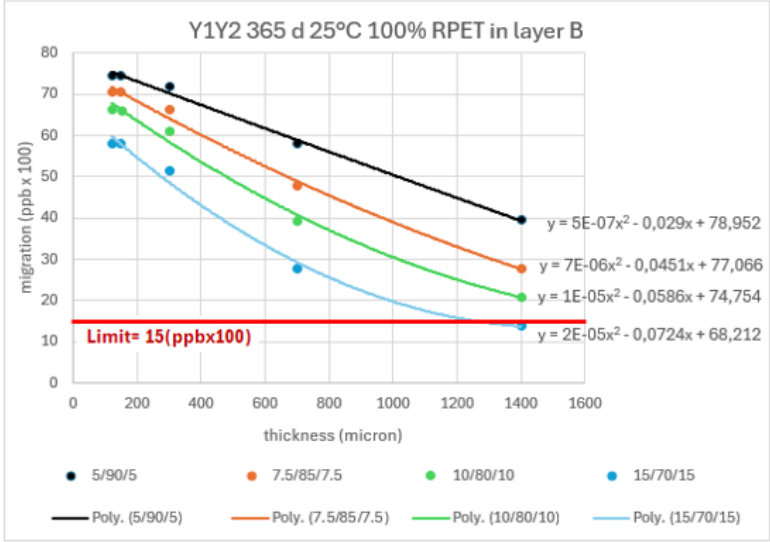



## Y1Y2 Configurations at 365 Days 25ºC



## Annex III -Substances with Molecular Weight less than 1000 Da, and relevant occurrence, found in the input material.

| Functional Barrier 3rd Monitoring Program | | | |
|---|---|---|---|
| October 10th 2024 | | | |
| **Annex III: substances in the input** | | | |
| substances in the input | cas nr | mol weight | occurence in the input/100 |
| 2-methyl-1,3-dioxolane | 497-26-7 | 88,0 | 0,95 |
| acetaldehyde | 75-07-0 | 44,1 | 0,80 |
| benzene | 71-43-2 | 78,0 | 0,78 |
| acetic acid | 64-19-7 | 60,1 | 0,69 |
| benzaldehyde | 100-52-7 | 106,0 | 0,64 |
| formic acid | 64-18-6 | 46,0 | 0,61 |
| acetic acid, ethyl ester | 141-78-6 | 88,1 | 0,60 |
| pet oligomers | n.a | | 0,59 |
| terephthalic acid | 100-21-0 | 166,1 | 0,58 |
| acetone | 67-64-1 | 58,0 | 0,57 |
| ethyleneglycol | 107-21-1 | 62,1 | 0,57 |
| ethanol | 64-17-5 | 46,1 | 0,57 |
| limonene | 138-86-3 | 136,0 | 0,54 |
| toluene | 108-88-3 | 92,0 | 0,54 |
| acetophenone | 98-86-2 | 120,0 | 0,52 |
| 2-pentyl-furan | 3777-69-3 | 138,0 | 0,52 |
| butyrolactone | 96-48-0 | 86,0 | 0,49 |
| tpa-eg oligomers | n.a | | 0,45 |
| phosphorous acid, tris(2,4-di-tert-butylphenyl)ester | 31570-04-4 | 646,9 | 0,40 |
| aibn | 78-67-1 | 164,0 | 0,40 |
| oleamide | 301-02-0 | 281,5 | 0,40 |
| xylenes | n.a | 106,0 | 0,39 |
| styrene | 100-42-5 | 104,2 | 0,39 |
| oxidized irgafos 168 | 95906-11-9 | 663,0 | 0,37 |
| 2,2-bis(4-hydroxyphenyl)propane | 80-05-7 | 228,3 | 0,37 |
| 2-[2-hydroxy-3,5-bis(1,1-dimethylbenzyl)phenyl]benzotriazole | 70321-86-7 | 447,0 | 0,37 |
| 2-ethyl-1-hexanol | 104-76-7 | 130,0 | 0,34 |
| 1,4-benzenedicarboxylic acid, bis(2-hydroxyethyl) ester | 959-26-2 | 254,1 | 0,33 |
| bis(2-ethylhexyl) sebacate | 122-62-3 | 427,0 | 0,30 |
| 1,2-ethanediol, monoacetate | 542-59-6 | 104,0 | 0,30 |
| aldehydes | n.a | | 0,30 |
| ketones | n.a | | 0,29 |
| 1-pentanol | 71-41-0 | 88,2 | 0,28 |
| γ-terpinene | 99-85-4 | 136,0 | 0,28 |
| p-cymene | 99-87-6 | 134,0 | 0,27 |
| ethylbenzene | 100-41-4 | 106,0 | 0,26 |
| 9,10-anthracenedione, 1,4-bis[(2-ethyl-6-methylphenyl)amino]- | 41611-76-1 | | 0,24 |
| d-limonene | 5989-27-5 | 136,1 | 0,23 |
| prob. dichloromethane | 75-09-2 | 84,0 | 0,23 |
| 3-((12-acetoxyoctadecanoyl)oxy)propane-1,2-diyl diacetate | 330198-91-9 | 500,3 | 0,23 |
| terephthalic acid, bis(2-ethylhexyl)ester | 6422-86-2 | | 0,22 |
| benzoic acid | 65-85-0 | 122,1 | 0,21 |
| 1-acetoxyacetone | 592-20-1 | 116,0 | 0,21 |
| 1,4-dioxane | 123-91-1 | 88,0 | 0,20 |
| hydrocarbons | n.a | 0,0 | 0,20 |
| phthalic acid, bis(2-ethylhexyl) ester | 117-81-7 | 390,6 | 0,17 |
| adipic acid, bis(2-ethylhexyl) ester | 103-23-1 | 370,0 | 0,17 |
| 1,2-ethanediol diformate | 629-15-2 | 118,0 | 0,17 |
| 1,2-ethanediol, monoformate | 628-35-3 | 90,0 | 0,17 |
| salicylic acid, methyl ester | 119-36-8 | | 0,16 |
| carboxylic acid | n.a | | 0,16 |
| hexanal | 66-25-1 | 100,0 | 0,16 |
| 1,4-benzenedicarboxaldehyde | 623-27-8 | 134,0 | 0,16 |
| palmitamide | 629-54-9 | 255,4 | 0,14 |
| 1-butanol | 71-36-3 | 74,1 | 0,14 |
| 4-methyl-3-pentenoic acid | 504-85-8 | 114,0 | 0,14 |

| Annex III: substances in the input | | | |
|---|---|---|---|
| **substances in the input** | **cas_nr** | **mol weight** | **occurence in the input/100** |
| 3,6,13,16-tetraoxatricyclo[16.2.2.2(8,11)]tetracosa-8,10,18,20,21,23-hexaene-2,7,12,17-tetrone | 1000398-77-0 | 384,1 | 0,14 |
| tpa-eg oligomers ** | n.a | | 0,13 |
| cyclic[tpa+eg]3+[ipa+eg] | n.a | 768,2 | 0,13 |
| cyclic[tpa+eg]2+[ipa+deg] | n.a | 634,8 | 0,13 |
| cyclic[tpa+eg]+[ipa+eg] | n.a | 384,1 | 0,13 |
| cyclic[tpa+deg]2 | n.a | 479,5 | 0,13 |
| δ-valerolactone | 542-28-9 | 100,0 | 0,12 |
| cyclic[tpa+eg]2+[ipa+eg] | n.a | 598,1 | 0,12 |
| benzyl acetate | 140-11-4 | 150,0 | 0,12 |
| nonanal | 124-19-6 | 142,0 | 0,11 |
| naphthalene | 91-20-3 | 128,0 | 0,11 |
| cyclic[tpa+eg]+[ipa+deg] | n.a | 428,1 | 0,11 |
| linear[tpa+eg]2+deg | n.a | 512,1 | 0,11 |
| 1,3-dioxolane | 646-06-0 | 74,1 | 0,11 |
| palmitic acid | 57-10-3 | 256,4 | 0,10 |
| isophthalaldehyde | 626-19-7 | 134,0 | 0,10 |
| phenol | 108-95-2 | 94,1 | 0,10 |
| octadecanoic acid, 2,3-bis(acetyloxy)propyl ester | 33599-07-4 | 442,3 | 0,10 |
| furfural | 98-01-1 | 96,0 | 0,10 |
| erucamide | 112-84-5 | 337,6 | 0,10 |
| cyclic[tpa+eg]4+[ipa+eg] | n.a | 960,2 | 0,10 |
| 2-ethylhexyl-acetate | 103-09-3 | 172,0 | 0,10 |
| 2,6-dimethyl-pyridine | 108-48-5 | 107,0 | 0,10 |
| 1-stearoylglycerol (1-monostearin) | 123-94-4 | 380,3 | 0,10 |
| 1-hydroxy-4-(p-toluidino)anthraquinone | 81-48-1 | 329,1 | 0,10 |
| tetrahydrofuran | 109-99-9 | 72,1 | 0,09 |
| 4(1h)-quinazolinone | 491-36-1 | 146,0 | 0,09 |
| linear[tpa+eg]3+eg | n.a | 660,1 | 0,08 |
| linear[tpa+eg]2 | n.a | 402,1 | 0,08 |
| isophthalic acid | 121-91-5 | | 0,08 |
| cyclic[tpa+eg]3+[ipa+deg] | n.a | 480,3 | 0,08 |
| cyclic[tpa+eg]+[tpa+deg]2 | | 686,2 | 0,08 |
| 2,4-dimethylfuran | 3710-43-8 | 96,0 | 0,08 |
| 1,2-ethanediol, monobenzoate | 94-33-7 | 166,1 | 0,08 |
| octanal | 124-13-0 | | 0,08 |
| linear[tpa+eg]3+deg | n.a | 380,3 | 0,08 |
| linear[tpa+eg]2+eg | n.a | 468,1 | 0,08 |
| heptanal | 111-71-7 | | 0,08 |
| cyclic[tpa+eg]4+[tpa+deg] | n.a | 1026,2 | 0,08 |
| 2-propenal | 107-02-8 | | 0,08 |
| 2-pentanone | 107-87-9 | | 0,08 |
| 1,2-ethanediol, diacetate | 111-55-7 | 146,0 | 0,08 |
| pentanal | 110-62-3 | | 0,07 |
| hexanoic acid | 142-62-1 | 116,0 | 0,07 |
| eucalyptol | 470-82-6 | 154,0 | 0,07 |
| 2-nonanone | 821-55-6 | | 0,07 |
| tri-n-butyl acetyl citrate | 77-90-7 | | 0,07 |
| phenol, 2,4-bis(1-methyl-1-phenylethyl)- | 2772-45-4 | 330,2 | 0,07 |
| cumene | 98-82-8 | 120,0 | 0,07 |
| benzonitrile, 2-amino- | 1885-29-6 | 118,1 | 0,07 |
| aldehydes c5-c11 | n.a | 44,0 | 0,07 |
| prob. 1-acetate-1,2-propanediol | 627-69-0 | 118,0 | 0,06 |
| methyl hydroxyacetate | 96-35-5 | | 0,06 |
| methyl formate | 107-31-3 | | 0,06 |
| cyclotetrasiloxane, octamethyl- | 556-67-2 | 296,1 | 0,06 |

| Annex III: substances in the input | | | |
|---|---|---|---|
| substances in the input | cas_nr | mol weight | occurence in the input/100 |
| acetic acid, methyl ester | 79-20-9 | | 0,06 |
| 4(1h)-quinazolinone, 2-methyl- | 1769-24-0 | 160,1 | 0,06 |
| 2-methyl-furan | 534-22-5 | 82,0 | 0,06 |
| stearic acid | 57-11-4 | 284,5 | 0,05 |
| solvent blue 104 | 116-75-6 | 474,2 | 0,05 |
| pet cyclic trimer | 7441-32-9 | 576,1 | 0,05 |
| nonylphenol ethoxylates (npeo5) | n.a | 459,3 | 0,05 |
| ketones c5-c10 | n.a | | 0,05 |
| butyric acid | 107-92-6 | 88,1 | 0,05 |
| bis(3,4-dimethylbenzylidene)sorbitol | 135861-56-2 | | 0,05 |
| benzene, 1,2,3-trimethyl- or isomer | 526-73-8 | 120,0 | 0,05 |
| acetic acid, butyl ester | 123-86-4 | | 0,05 |
| 2-decanone | 693-54-9 | | 0,05 |
| 1,1,1-trimethylolpropane | 77-99-6 | 134,0 | 0,05 |
| triphenylphosphine oxide | 791-28-6 | 278,1 | 0,05 |
| propanal, 2-methyl- | 78-84-2 | | 0,05 |
| methacrolein | 78-85-3 | | 0,05 |
| dimethylsilanediol | 1066-42-8 | | 0,05 |
| caprolactone | 502-44-3 | | 0,05 |
| butyraldehyde | 123-72-8 | 72,1 | 0,05 |
| benzoic acid, 4-methyl-, 2-hydroxyethyl ester | 28129-15-9 | 180,1 | 0,05 |
| aldehydes c5-c10 | n.a | 44,0 | 0,05 |
| 9-octadecenoic acid (z)-, 2,3-bis(acetyloxy)propyl ester | 55401-64-4 | | 0,05 |
| 2-hexanone | 591-78-6 | | 0,05 |
| 2-heptanone | 110-43-0 | | 0,05 |
| 2-butenal | 4170-30-3 | | 0,05 |
| 2-butanone | 78-93-3 | | 0,05 |
| 2,5-bis(5-tert-butyl-2-benzoxazolyl)thiophene | 7128-64-5 | 430,0 | 0,05 |
| 1,3,5-trimethyl-benzene | 108-67-8 | 120,0 | 0,05 |
| 1,2-cyclohexanedicarboxylic acid, diisononyl ester | 166412-78-8 | | 0,05 |
| undecanal | 112-44-7 | | 0,04 |
| thiodipropionic acid, didodecyl ester | 123-28-4 | 514,9 | 0,04 |
| propyl-benzene | 103-65-1 | 120,0 | 0,04 |
| propionaldehyde | 123-38-6 | | 0,04 |
| pet cyclic dimer | 24388-68-9 | 384,1 | 0,04 |
| p/o-xylene | 106-42-3/95- | 106,0 | 0,04 |
| o-phthalic acid | 88-99-3 | | 0,04 |
| octadecanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester | 55401-62-2 | | 0,04 |
| hexadecanoic acid, hexadecyl ester | 540-10-3 | | 0,04 |
| furan | 110-00-9 | | 0,04 |
| ftalan dietylu | 84-66-2 | 222,1 | 0,04 |
| dioctyl adipate | 123-79-5 | 370,3 | 0,04 |
| cyclopentanone | 120-92-3 | 84,0 | 0,04 |
| cyclohexane | 110-82-7 | 84,0 | 0,04 |
| c[eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | n.a | | 0,04 |
| c[eg/pa/eg/pa/eg/pa] pa=phthalic acid eg=ethylene glycol | n.a | | 0,04 |
| c[eg/pa/eg/pa/eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | n.a | | 0,04 |
| c[deg/pa/eg/pa/eg/pa/eg/pa] pa=phthalic acid eg=ethylene glycol deg=diethylene glycol | n.a | | 0,04 |
| c[deg/pa/deg/pa] deg= diethylen glycol pa= phthalic acid | n.a | | 0,04 |
| benzene, 1-ethyl-4-methyl- or isomer | 622-96-8 | 120,0 | 0,04 |
| aldehydes c5-c12 | n.a | | 0,04 |
| acrylic acid, dodecyl ester | 2156-97-0 | | 0,04 |
| 2-methylbutyl acetate | 624-41-9 | 130,0 | 0,04 |
| 2-aminobenzamide | 88-68-6 | 368,0 | 0,04 |
| 2,4-di-tert-butylphenol | 96-76-4 | | 0,04 |
| 2(3h)-furanone, 5-ethyldihydro- | 695-06-7 | | 0,04 |
| 1-propanol | 71-23-8 | 60,1 | 0,04 |
| triethylene glycol monobutyl ether | 143-22-6 | 206,2 | 0,04 |
| tetradecanoic acid, hexadecyl ester | 2599-01-1 | | 0,04 |
| succinic anhydride | 108-30-5 | 100,0 | 0,04 |
| solvent green 3 | 128-80-3 | 418,5 | 0,04 |
| probable pet oligomer (dimer ether) | n.a | | 0,04 |
| probable pet oligomer (cyclic dimer) | n.a | | 0,04 |
| n-propyl acetate | 109-60-4 | 102,0 | 0,04 |
| myristyl myristate | 3234-85-3 | 424,4 | 0,04 |
| isothymol | 499-75-2 | 150,0 | 0,04 |
| hexamethyl cyclotrisiloxane | 541-05-9 | | 0,04 |
| hexadecanoic acid, octadecyl ester | 2598-99-4 | | 0,04 |
| ethylene terephthalate cyclic tetramer | 16104-96-4 | 768,7 | 0,04 |

| Annex III: substances in the input | | | |
|---|---|---|---|
| substances in the input | cas_nr | mol weight | occurence in the input/100 |
| ethylene (tere-,iso-)phthalate cyclic pentamer_pto | 16104-97-5 | 960,2 | 0,04 |
| eicosanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester | 55429-68-0 | | 0,04 |
| dof / 2-ethylhexyl fumarate | 141-02-6 | 340,3 | 0,04 |
| dihydro-5-methyl-2(3h)-furanone | 108-29-2 | 100,0 | 0,04 |
| decanal | 112-31-2 | | 0,04 |
| cyclopentasiloxane, decamethyl- | 541-02-6 | 370,1 | 0,04 |
| carboxylic acids | n.a | | 0,04 |
| c[eg/pa/eg/pa/eg/pa/eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | n.a | | 0,04 |
| c[deg/pa/eg/pa] pa=phthalic acid deg=diethylen glycol eg=ethylen glycol | n.a | 428,1 | 0,04 |
| c[deg/pa/eg/pa/eg/pa] pa=phthalic acid deg=diethylen glycol eg=ethylen glycol | n.a | 620,2 | 0,04 |
| butyl carbitol | 112-34-5 | 184,1 | 0,04 |
| 4-amino-benzonitrile | 873-74-5 | 118,0 | 0,04 |
| 4-(1-methylethyl)-benzaldehyde | 122-03-2 | 148,0 | 0,04 |
| 2,2'-(1,4-phenylene)bis[4H-3,1-benzoxazin-4-one] | 18600-59-4 | 369,0 | 0,04 |
| 2-(2-hydroxypropoxy)-1-propanol | 106-62-7 | 134,0 | 0,04 |
| 1-octanol | 111-87-5 | 130,2 | 0,04 |
| 1-ethyl-3-methyl-benzene | 620-14-4 | 120,0 | 0,04 |
| p-toluic acid, 5-tridecyl ester | n.a | 318,3 | 0,03 |
| prob. pyridine | 110-86-1 | 79,0 | 0,03 |
| prob. 2,5-dimethyl-furan | 625-86-5 | 96,0 | 0,03 |
| pentaerythritol | 115-77-5 | 136,2 | 0,03 |
| palmitoleamide | 106010-22-4 | 253,2 | 0,03 |
| octadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 621-61-4 | 358,3 | 0,03 |
| nonylphenol ethoxylates (npeo7) | n.a | 550,3 | 0,03 |
| n-hexane | 110-54-3 | 86,0 | 0,03 |
| methacrylic acid, methyl ester | 80-62-6 | 100,1 | 0,03 |
| maleic anhydride | 108-31-6 | 98,1 | 0,03 |
| linoleic acid | 60-33-3 | | 0,03 |
| linear[tpa+eg]3 | n.a | 594,1 | 0,03 |
| linear[tpa+eg]+deg | n.a | 320,1 | 0,03 |
| l[eg/pa/eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | n.a | | 0,03 |
| hexyl 2-(1-hexoxy-1-oxopropan-2-yl)sulfanylpropanoate | n.a | 346,2 | 0,03 |
| hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 23470-00-0 | 330,3 | 0,03 |
| hexadecanoic acid, 2,3-bis(acetyloxy)propyl ester | 55268-70-7 | 414,3 | 0,03 |
| hexacosane | 630-01-3 | 366,4 | 0,03 |
| cyclohexasiloxane, dodecamethyl- | 540-97-6 | 444,1 | 0,03 |
| 2-octanone | 111-13-7 | | 0,03 |
| 2-n-butyl furan | 4466-24-4 | 124,0 | 0,03 |
| 2-chloroethyl benzoate | 939-55-9 | 184,0 | 0,03 |
| 2,2'-oxybis-1-propanol | 108-61-2 | 134,0 | 0,03 |
| 1-octene | 111-66-0 | 112,2 | 0,03 |
| 1-octadecanol | 112-92-5 | 270,3 | 0,03 |
| 1-methyl-3-propyl-benzene | 1074-43-7 | 134,0 | 0,03 |
| 1-hexadecanol | 36653-82-4 | 242,5 | 0,03 |
| 1,3-dipropylene glycol | 2396-61-4 | 134,0 | 0,03 |
| (m-z : 429.1-104.0-208.1-385.1); possible cyclic oligomer: (iso-tere)phathalic acid - ethylene glycol - (iso-tere)phathalic acid - diethylene glycol | n.a | 428,1 | 0,03 |
| (m-z : 385.2-296.1-104.0-149.1-341.1) ;possible cyclic oligomer: (iso-tere)phathalic acid - ethylene glycol - (iso-tere)phathalic acid - ethylene glycol | n.a | 384,1 | 0,03 |
| (m-z : 385.2-104.0-296.1-341.1-429.1) ;possible cyclic oligomer: (iso-tere)phathalic acid - ethylene glycol - (iso-tere)phathalic acid - ethylene glycol | n.a | 384,1 | 0,03 |
| (m-z : 341.1-296.1-104.0-324.1-236.1-354.1-384.1) ; possible linear oligomer: (iso-tere)phathalic acid - ethylene glycol - (iso-tere)phathalic acid - ethylene glycol | n.a | 490,1 | 0,03 |
| (m-z : 296.1-341.1-104.0-324.1-384.1); possible linear oligomer: (iso-tere)phathalic acid - ethylene glycol - (iso-tere)phathalic acid - ethylene glycol | n.a | 490,1 | 0,03 |
| (m-z : 193.0-149.0-104.0-175.0); possible linear oligomer: terephathalic acid - ethylene glycol | n.a | | 0,03 |
| (m-z : 130.0-117.0-371.3-239.2) | n.a | | 0,03 |

## Annex IV -Substances with Molecular Weight less than 1000 Da, and relevant occurrence, found in the output material.

| Functional Barrier 3rd Monitoring Program | | | |
|---|---|---|---|
| October 10th 2024 | | | |
| **ANNEX IV a : substances in output for technology configuration X1X2W** | | | |
| **substance** | **cas_nr** | **mw** | **occurence in output** |
| benzene | 71-43-2 | 78 | 0,93 |
| 2-methyl-1,3-dioxolane | 497-26-7 | 88 | 0,91 |
| acetaldehyde | 75-07-0 | 44,05 | 0,81 |
| acetic acid | 64-19-7 | 60,05 | 0,69 |
| terephthalic acid | 100-21-0 | 166,13 | 0,61 |
| pet oligomers | | | 0,61 |
| acetone | 67-64-1 | 58 | 0,61 |
| formic acid | 64-18-6 | 46 | 0,58 |
| ethyleneglycol | 107-21-1 | 62,07 | 0,58 |
| toluene | 108-88-3 | 92 | 0,55 |
| benzaldehyde | 100-52-7 | 106,04 | 0,54 |
| limonene | 138-86-3 | 136 | 0,5 |
| acetic acid, ethyl ester | 141-78-6 | | 0,5 |
| styrene | 100-42-5 | 104,15 | 0,47 |
| tpa-eg oligomers | | | 0,45 |
| acetophenone | 98-86-2 | 120 | 0,42 |
| 2,2-bis(4-hydroxyphenyl)propane | 80-05-7 | 228,29 | 0,4 |
| 2-[2-hydroxy-3,5-bis(1,1-dimethylbenzyl)phenyl]benzotriazole | 70321-86-7 | 447 | 0,39 |
| 2-pentyl-furan | 3777-69-3 | 138 | 0,36 |
| 1,4-benzenedicarboxylic acid, bis(2-hydroxyethyl) ester | 959-26-2 | 254,08 | 0,36 |
| 1,2-ethanediol, monoacetate | 542-59-6 | 104 | 0,31 |
| xylenes | | 106 | 0,3 |
| aldehydes | | | 0,29 |
| aibn | 78-67-1 | 164 | 0,29 |
| ketones | | | 0,26 |
| 1,4-dioxane | 123-91-1 | 88 | 0,26 |
| butyrolactone | 96-48-0 | 86 | 0,25 |
| 9,10-anthracenedione, 1,4-bis[(2-ethyl-6-methylphenyl)amino]- | 41611-76-1 | | 0,25 |
| 3-((12-acetoxyoctadecanoyl)oxy)propane-1,2-diyl diacetate | 330198-91-9 | 500,34 | 0,25 |
| 1-pentanol | 71-41-0 | 88,15 | 0,23 |
| 1,2-ethanediol, monoformate | 628-35-3 | 90 | 0,23 |
| terephthalic acid, bis(2-ethylhexyl)ester | 6422-86-2 | | 0,21 |
| prob. dichloromethane | 75-09-2 | 84 | 0,21 |
| adipic acid, bis(2-ethylhexyl) ester | 103-23-1 | 370 | 0,2 |
| 4-methyl-3-pentenoic acid | 504-85-8 | 114 | 0,2 |
| oxidized irgafos 168 | 95906-11-9 | 663 | 0,19 |
| d-limonene | 5989-27-5 | 136,13 | 0,19 |
| bis(2-ethylhexyl) sebacate | 122-62-3 | 427 | 0,19 |
| phosphorous acid, tris(2,4-di-tert-butylphenyl)ester | 31570-04-4 | 646,94 | 0,17 |
| naphthalene | 91-20-3 | 128 | 0,17 |
| hydrocarbons | | 0 | 0,17 |
| tpa-eg oligomers ** | | | 0,14 |
| phthalic acid, bis(2-ethylhexyl) ester | 117-81-7 | 390,6 | 0,14 |
| 3,6,13,16-tetraoxatricyclo[16.2.2.2(8,11)]tetracosa-8,10,18,20,21,23-hexaene-2,7,12,17-tetrone | 1000398-77-( | 384,09 | 0,14 |
| furfural | 98-01-1 | 96 | 0,13 |
| ethylbenzene | 100-41-4 | 106 | 0,13 |
| ethanol | 64-17-5 | 46,07 | 0,13 |
| cyclic[tpa+deg]2 | | 479,46 | 0,13 |
| cyclic[tpa+eg]2+[ipa+eg] | | 598,11 | 0,13 |
| cyclic[tpa+eg]2+[ipa+deg] | | 634,81 | 0,13 |

## ANNEX IV a : substances in output for technology configuration X1X2W

| substance | cas_nr | mw | occurence in output |
|---|---|---|---|
| cyclic[tpa+eg]+[ipa+eg] | | 384,08 | 0,13 |
| cyclic[tpa+eg]3+[ipa+eg] | | 768,17 | 0,12 |
| cyclic[tpa+eg]+[tpa+deg]2 | | 686,16 | 0,12 |
| cyclic[tpa+eg]+[ipa+deg] | | 428,11 | 0,12 |
| 4(1h)-quinazolinone | 491-36-1 | 146,05 | 0,12 |
| linear[tpa+eg]2+deg | | 512,13 | 0,11 |
| 1-hydroxy-4-(p-toluidino)anthraquinone | 81-48-1 | 329,11 | 0,11 |
| phenol | 108-95-2 | 94,11 | 0,1 |
| oleamide | 301-02-0 | 281,5 | 0,1 |
| nonanal | 124-19-6 | 142 | 0,1 |
| linear[tpa+eg]2+eg | | 468,1 | 0,1 |
| cyclopentanone | 120-92-3 | 84 | 0,1 |
| cyclic[tpa+eg]3+[ipa+deg] | | 480,31 | 0,1 |
| 1,2-ethanediol diformate | 629-15-2 | 118 | 0,1 |
| hexanal | 66-25-1 | 100 | 0,09 |
| cyclic[tpa+eg]4+[ipa+eg] | | 960,21 | 0,09 |
| benzoic acid | 65-85-0 | 122,12 | 0,09 |
| 2-ethyl-1-hexanol | 104-76-7 | 130 | 0,09 |
| octadecanoic acid, 2,3-bis(acetyloxy)propyl ester | 33599-07-4 | 442,33 | 0,09 |
| linear[tpa+eg]2 | | 402,1 | 0,09 |
| erucamide | 112-84-5 | 337,59 | 0,09 |
| cyclic[tpa+eg]4+[tpa+deg] | | 1.026,22 | 0,09 |
| 1,2-ethanediol, monobenzoate | 94-33-7 | 166,06 | 0,09 |
| palmitic acid | 57-10-3 | 256,43 | 0,08 |
| linear[tpa+eg]3+deg | | 380,29 | 0,08 |
| 2,6-dimethyl-pyridine | 108-48-5 | 107 | 0,08 |
| 1-stearoylglycerol (1-monostearin) | 123-94-4 | 380,29 | 0,08 |
| methacrylic acid, methyl ester | 80-62-6 | 100,12 | 0,07 |
| 9-octadecenoic acid (z)-, 2,3-bis(acetyloxy)propyl ester | 55401-64-4 | | 0,07 |
| isophthalaldehyde | 626-19-7 | 134,04 | 0,07 |
| bis(3,4-dimethylbenzylidene)sorbitol | 135861-56-2 | | 0,07 |
| acetic acid, methyl ester | 79-20-9 | | 0,07 |
| 1-butanol | 71-36-3 | 74,12 | 0,07 |
| 1,4-benzenedicarboxaldehyde | 623-27-8 | 134 | 0,07 |
| tri-n-butyl acetyl citrate | 77-90-7 | | 0,06 |
| stearic acid | 57-11-4 | 284,49 | 0,06 |
| pentanal | 110-62-3 | | 0,06 |
| nonylphenol ethoxylates (npeo5) | | 459,29 | 0,06 |
| linear[tpa+eg]3 | | 594,14 | 0,06 |
| heptanal | 111-71-7 | | 0,06 |
| decanal | 112-31-2 | | 0,06 |
| carboxylic acid | | | 0,06 |
| 4(1h)-quinazolinone, 2-methyl- | 1769-24-0 | 160,06 | 0,06 |
| solvent blue 104 | 116-75-6 | 474,23 | 0,06 |
| linear[tpa+eg]3+eg | | 660,15 | 0,06 |
| isopropyl myristate | 110-27-0 | 270 | 0,06 |
| hexamethyl cyclotrisiloxane | 541-05-9 | | 0,06 |
| furan | 110-00-9 | | 0,06 |
| dimethylsilanediol | 1066-42-8 | | 0,06 |
| aldehydes c6-c10 | | | 0,06 |
| 2-propenal | 107-02-8 | | 0,06 |
| 2-butenal | 4170-30-3 | | 0,06 |
| 1-propene-1,2,3-tricarboxylic acid, tributyl ester | 7568-58-3 | | 0,06 |
| 1-hexadecanol | 36653-82-4 | 242,45 | 0,06 |
| α-methylstyrene | 98-83-9 | | 0,05 |
| thiodipropionic acid, didodecyl ester | 123-28-4 | 514,86 | 0,05 |
| phenol, 2,4-bis(1-methyl-1-phenylethyl)- | 2772-45-4 | 330,2 | 0,05 |
| pet cyclic trimer | 7441-32-9 | 576,13 | 0,05 |
| octadecanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester | 55401-62-2 | | 0,05 |
| linear[tpa+eg]+deg | | 320,09 | 0,05 |

## ANNEX IV a : substances in output for technology configuration X1X2W

| substance | cas_nr | mw | occurence in output |
|---|---|---|---|
| citric acid, triethyl ester | 77-93-0 | | 0,05 |
| 4-formyl-benzonitrile | 105-07-7 | 131 | 0,05 |
| 2-pentanone | 107-87-9 | | 0,05 |
| 2,5-bis(5-tert-butyl-2-benzoxazolyl)thiophene | 7128-64-5 | 430 | 0,05 |
| 2,4-di-tert-butylphenol | 96-76-4 | | 0,05 |
| 1,3-dioxolane | 646-06-0 | 74,08 | 0,05 |
| solvent green 3 | 128-80-3 | 418,5 | 0,04 |
| pet cyclic dimer | 24388-68-9 | 384,08 | 0,04 |
| palmitamide | 629-54-9 | 255,44 | 0,04 |
| methyl formate | 107-31-3 | | 0,04 |
| ketones c5-c11 | | | 0,04 |
| isophthalic acid | 121-91-5 | | 0,04 |
| heptane | 142-82-5 | 100 | 0,04 |
| dioctyl adipate | 123-79-5 | 370,31 | 0,04 |
| dihydro-5-methyl-2(3h)-furanone | 108-29-2 | 100 | 0,04 |
| cyclopentasiloxane, decamethyl- | 541-02-6 | 370,09 | 0,04 |
| c[eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | | | 0,04 |
| c[eg/pa/eg/pa/eg/pa] pa=phthalic acid eg=ethylene glycol | | | 0,04 |
| c[eg/pa/eg/pa/eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | | | 0,04 |
| c[eg/pa/eg/pa/eg/pa/eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | | | 0,04 |
| c[deg/pa/eg/pa/eg/pa/eg/pa] pa=phthalic acid eg=ethylene glycol deg=diethylene glycol | | | 0,04 |
| c[deg/pa/deg/pa] deg= diethylen glycol pa= phthalic acid | | | 0,04 |
| benzonitrile, 2-amino- | 1885-29-6 | 118,05 | 0,04 |
| benzoic acid, 4-methyl-, 2-hydroxyethyl ester | 28129-15-9 | 180,08 | 0,04 |
| aldehydes c5-c11 | | 44 | 0,04 |
| 2-hexanone | 591-78-6 | | 0,04 |
| 2,4-dimethylfuran | 3710-43-8 | 96 | 0,04 |
| triphenylphosphine oxide | 791-28-6 | 278,09 | 0,04 |
| tetrahydrofuran | 109-99-9 | 72,11 | 0,04 |
| stearamide | 124-26-5 | 283,5 | 0,04 |
| hexanoic acid | 142-62-1 | 116 | 0,04 |
| hexacosane | 630-01-3 | 366,4 | 0,04 |
| ethylene terephthalate cyclic tetramer | 16104-96-4 | 768,67 | 0,04 |
| ethylene carbonate | 96-49-1 | 88,06 | 0,04 |
| dodecane | 112-40-3 | 170 | 0,04 |
| cyclotetrasiloxane, octamethyl- | 556-67-2 | 296,08 | 0,04 |
| c[deg/pa/eg/pa] pa=phthalic acid deg=diethylen glycol eg=ethylen glycol | | 428,11 | 0,04 |
| c[deg/pa/eg/pa/eg/pa] pa=phthalic acid deg=diethylen glycol eg=ethylen glycol | | 620,15 | 0,04 |
| bis-gma / bisphenol a glycidylmethacrylate | 1565-94-2 | 843,24 | 0,04 |
| aldehydes c6-c12 | | | 0,04 |
| 2-propanol | 67-63-0 | 60,1 | 0,04 |
| 2-heptanone | 110-43-0 | | 0,04 |
| 2,2'-(1,4-phenylene)bis[4H-3,1-benzoxazin-4-one] | 18600-59-4 | 369 | 0,04 |
| 1-decanol, 2-hexyl- | 2425-77-6 | | 0,04 |
| 1-acetoxyacetone | 592-20-1 | 116 | 0,04 |
| unknown substance [m/z: 341.0, 208.0, 236.0] | | 0 | 0,03 |
| succinic anhydride | 108-30-5 | 100 | 0,03 |
| p-toluic acid, 5-tridecyl ester | | 318,3 | 0,03 |
| probable pet oligomer (dimer ether) | | | 0,03 |
| probable pet oligomer (cyclic dimer) | | | 0,03 |
| polyethyleneglycol (eo = 1-50) ethers of linear and branched primary (c 8-c 22) alcohols | | | 0,03 |
| p-cymene | 99-87-6 | 134 | 0,03 |
| octanal + d-limonene | 124-13-0 + 5989-27-5 | | 0,03 |
| octadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 621-61-4 | 358,3 | 0,03 |
| n-butylbenzenesulphonamide (n-butylbenzenesulfonamide) | 3622-84-2 | 213,08 | 0,03 |
| myristic acid | 544-63-8 | 228,38 | 0,03 |
| methyl hydroxyacetate | 96-35-5 | | 0,03 |
| l[eg/pa/eg/pa/eg] eg=ethylen glycol pa=phthalic acid | | | 0,03 |
| ketones c5-c8 | | | 0,03 |
| hexyl 2-(1-hexoxy-1-oxopropan-2-yl)sulfanylpropanoate | | 346,22 | 0,03 |
| hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 23470-00-0 | 330,28 | 0,03 |
| heptane, 2,2,4,6,6-pentamethyl- | 13475-82-6 | 170 | 0,03 |
| eucalyptol | 470-82-6 | 154 | 0,03 |
| ethylene (tere-,iso-)phthalate cyclic pentamer_pto | 16104-97-5 | 960,21 | 0,03 |
| ethoxylated bisphenol a diacrylate | 64401-02-1 | 446,17 | 0,03 |
| eicosanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester | 55429-68-0 | | 0,03 |
| cyclohexasiloxane, dodecamethyl- | 540-97-6 | 444,11 | 0,03 |
| carboxylic acids | | | 0,03 |
| carbonic acid, eicosyl vinyl ester | 1000382-54-3 | 368 | 0,03 |
| caprylic acid | 124-07-2 | 144,22 | 0,03 |
| caprolactone | 502-44-3 | | 0,03 |
| butyraldehyde | 123-72-8 | 72,11 | 0,03 |
| aldehydes c6-c9 | | | 0,03 |
| acrylic acid, dodecyl ester | 2156-97-0 | | 0,03 |
| 3,3'-dimetoxy-benzidin | 119-90-4 | 408,29 | 0,03 |
| 2-octanone | 111-13-7 | | 0,03 |
| 2-ethylhexyl-acetate | 103-09-3 | 172 | 0,03 |
| 2-butanone | 78-93-3 | | 0,03 |
| (m-z : 193.0-149.0-104.0-175.0); possible linear oligomer: terephathalic acid - ethylene glycol | | | 0,03 |
| (m-z : 130.0-117.0-371.3-239.2) | | | 0,03 |

## ANNEX IV a : substances in output for technology configuration X1X2W

| substance | cas_nr | mw | occurence in output |
|---|---|---|---|
| citric acid, triethyl ester | 77-93-0 | | 0,05 |
| 4-formyl-benzonitrile | 105-07-7 | 131 | 0,05 |
| 2-pentanone | 107-87-9 | | 0,05 |
| 2,5-bis(5-tert-butyl-2-benzoxazolyl)thiophene | 7128-64-5 | 430 | 0,05 |
| 2,4-di-tert-butylphenol | 96-76-4 | | 0,05 |
| 1,3-dioxolane | 646-06-0 | 74,08 | 0,05 |
| solvent green 3 | 128-80-3 | 418,5 | 0,04 |
| pet cyclic dimer | 24388-68-9 | 384,08 | 0,04 |
| palmitamide | 629-54-9 | 255,44 | 0,04 |
| methyl formate | 107-31-3 | | 0,04 |
| ketones c5-c11 | | | 0,04 |
| isophthalic acid | 121-91-5 | | 0,04 |
| heptane | 142-82-5 | 100 | 0,04 |
| dioctyl adipate | 123-79-5 | 370,31 | 0,04 |
| dihydro-5-methyl-2(3h)-furanone | 108-29-2 | 100 | 0,04 |
| cyclopentasiloxane, decamethyl- | 541-02-6 | 370,09 | 0,04 |
| c[eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | | | 0,04 |
| c[eg/pa/eg/pa/eg/pa] pa=phthalic acid eg=ethylene glycol | | | 0,04 |
| c[eg/pa/eg/pa/eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | | | 0,04 |
| c[eg/pa/eg/pa/eg/pa/eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | | | 0,04 |
| c[deg/pa/eg/pa/eg/pa/eg/pa] pa=phthalic acid eg=ethylene glycol deg=diethylene glycol | | | 0,04 |
| c[deg/pa/deg/pa] deg= diethylen glycol pa= phthalic acid | | | 0,04 |
| benzonitrile, 2-amino- | 1885-29-6 | 118,05 | 0,04 |
| benzoic acid, 4-methyl-, 2-hydroxyethyl ester | 28129-15-9 | 180,08 | 0,04 |
| aldehydes c5-c11 | | 44 | 0,04 |
| 2-hexanone | 591-78-6 | | 0,04 |
| 2,4-dimethylfuran | 3710-43-8 | 96 | 0,04 |
| triphenylphosphine oxide | 791-28-6 | 278,09 | 0,04 |
| tetrahydrofuran | 109-99-9 | 72,11 | 0,04 |
| stearamide | 124-26-5 | 283,5 | 0,04 |
| hexanoic acid | 142-62-1 | 116 | 0,04 |
| hexacosane | 630-01-3 | 366,4 | 0,04 |
| ethylene terephthalate cyclic tetramer | 16104-96-4 | 768,67 | 0,04 |
| ethylene carbonate | 96-49-1 | 88,06 | 0,04 |
| dodecane | 112-40-3 | 170 | 0,04 |
| cyclotetrasiloxane, octamethyl- | 556-67-2 | 296,08 | 0,04 |
| c[deg/pa/eg/pa] pa=phthalic acid deg=diethylen glycol eg=ethylen glycol | | 428,11 | 0,04 |
| c[deg/pa/eg/pa/eg/pa] pa=phthalic acid deg=diethylen glycol eg=ethylen glycol | | 620,15 | 0,04 |
| bis-gma / bisphenol a glycidylmethacrylate | 1565-94-2 | 843,24 | 0,04 |
| aldehydes c6-c12 | | | 0,04 |
| 2-propanol | 67-63-0 | 60,1 | 0,04 |
| 2-heptanone | 110-43-0 | | 0,04 |
| 2,2'-(1,4-phenylene)bis[4H-3,1-benzoxazin-4-one] | 18600-59-4 | 369 | 0,04 |
| 1-decanol, 2-hexyl- | 2425-77-6 | | 0,04 |
| 1-acetoxyacetone | 592-20-1 | 116 | 0,04 |
| unknown substance [m/z: 341.0, 208.0, 236.0] | | 0 | 0,03 |
| succinic anhydride | 108-30-5 | 100 | 0,03 |
| p-toluic acid, 5-tridecyl ester | | 318,3 | 0,03 |
| probable pet oligomer (dimer ether) | | | 0,03 |
| probable pet oligomer (cyclic dimer) | | | 0,03 |
| polyethyleneglycol (eo = 1-50) ethers of linear and branched primary (c 8-c 22) alcohols | | | 0,03 |
| p-cymene | 99-87-6 | 134 | 0,03 |
| octanal + d-limonene | 124-13-0 + 5989-27-5 | | 0,03 |
| octadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 621-61-4 | 358,3 | 0,03 |
| n-butylbenzenesulphonamide (n-butylbenzenesulfonamide) | 3622-84-2 | 213,08 | 0,03 |
| myristic acid | 544-63-8 | 228,38 | 0,03 |
| methyl hydroxyacetate | 96-35-5 | | 0,03 |
| i[eg/pa/eg/pa/eg] eg=ethylen glycol pa=phthalic acid | | | 0,03 |
| ketones c5-c8 | | | 0,03 |
| hexyl 2-(1-hexoxy-1-oxopropan-2-yl)sulfanylpropanoate | | 346,22 | 0,03 |

| ANNEX IV a : substances in output for technology configuration X1X2W | | | |
|---|---|---|---|
| **substance** | **cas_nr** | **mw** | **occurence in output** |
| hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 23470-00-0 | 330,28 | 0,03 |
| heptane, 2,2,4,6,6-pentamethyl- | 13475-82-6 | 170 | 0,03 |
| eucalyptol | 470-82-6 | 154 | 0,03 |
| ethylene (tere-,iso-)phthalate cyclic pentamer_pto | 16104-97-5 | 960,21 | 0,03 |
| ethoxylated bisphenol a diacrylate | 64401-02-1 | 446,17 | 0,03 |
| eicosanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester | 55429-68-0 | | 0,03 |
| cyclohexasiloxane, dodecamethyl- | 540-97-6 | 444,11 | 0,03 |
| carboxylic acids | | | 0,03 |
| carbonic acid, eicosyl vinyl ester | 1000382-54-3 | 368 | 0,03 |
| caprylic acid | 124-07-2 | 144,22 | 0,03 |
| caprolactone | 502-44-3 | | 0,03 |
| butyraldehyde | 123-72-8 | 72,11 | 0,03 |
| aldehydes c6-c9 | | | 0,03 |
| acrylic acid, dodecyl ester | 2156-97-0 | | 0,03 |
| 3,3'-dimetoxy-benzidin | 119-90-4 | 408,29 | 0,03 |
| 2-octanone | 111-13-7 | | 0,03 |
| 2-ethylhexyl-acetate | 103-09-3 | 172 | 0,03 |
| 2-butanone | 78-93-3 | | 0,03 |
| (m-z : 193.0-149.0-104.0-175.0); possible linear oligomer: terephathalic acid - ethylene glycol | | | 0,03 |
| (m-z : 130.0-117.0-371.3-239.2) | | | 0,03 |

# Functional Barrier 3rd Monitoring Program

October 10th 2024

## ANNEX IVb: substances in output for technology configuration Y1Y2

| substance | cas_nr | mw | occurence_ in output/100 |
|---|---|---|---|
| benzene | 71-43-2 | 78 | 0,93 |
| 2-methyl-1,3-dioxolane | 497-26-7 | 88 | 0,91 |
| acetaldehyde | 75-07-0 | 44,05 | 0,81 |
| acetic acid | 64-19-7 | 60,05 | 0,69 |
| terephthalic acid | 100-21-0 | 166,13 | 0,61 |
| pet oligomers | n.a | n.a | 0,61 |
| acetone | 67-64-1 | 58 | 0,61 |
| formic acid | 64-18-6 | 46 | 0,58 |
| ethyleneglycol | 107-21-1 | 62,07 | 0,58 |
| toluene | 108-88-3 | 92 | 0,55 |
| benzaldehyde | 100-52-7 | 106,04 | 0,54 |
| limonene | 138-86-3 | 136 | 0,50 |
| acetic acid, ethyl ester | 141-78-6 | | 0,50 |
| styrene | 100-42-5 | 104,15 | 0,47 |
| tpa-eg oligomers | n.a | n.a | 0,45 |
| acetophenone | 98-86-2 | 120 | 0,42 |
| 2,2-bis(4-hydroxyphenyl)propane | 80-05-7 | 228,29 | 0,40 |
| 2-[2-hydroxy-3,5-bis(1,1-dimethylbenzyl)phenyl]benzotriazole | 70321-86-7 | 447 | 0,39 |
| 2-pentyl-furan | 3777-69-3 | 138 | 0,36 |
| 1,4-benzenedicarboxylic acid, bis(2-hydroxyethyl) ester | 959-26-2 | 254,08 | 0,36 |
| 1,2-ethanediol, monoacetate | 542-59-6 | 104 | 0,31 |
| xylenes | n.a | 106 | 0,30 |
| aldehydes | n.a | n.a | 0,29 |
| aibn | 78-67-1 | 164 | 0,29 |
| ketones | n.a | n.a | 0,26 |
| 1,4-dioxane | 123-91-1 | 88 | 0,26 |
| butyrolactone | 96-48-0 | 86 | 0,25 |
| 9,10-anthracenedione, 1,4-bis[(2-ethyl-6-methylphenyl)amino]- | 41611-76-1 | | 0,25 |
| 3-((12-acetoxyoctadecanoyl)oxy)propane-1,2-diyl diacetate | 330198-91-9 | 500,34 | 0,25 |
| 1-pentanol | 71-41-0 | 88,15 | 0,23 |
| 1,2-ethanediol, monoformate | 628-35-3 | 90 | 0,23 |
| terephthalic acid, bis(2-ethylhexyl)ester | 6422-86-2 | | 0,21 |
| prob. dichloromethane | 75-09-2 | 84 | 0,21 |
| adipic acid, bis(2-ethylhexyl) ester | 103-23-1 | 370 | 0,20 |
| 4-methyl-3-pentenoic acid | 504-85-8 | 114 | 0,20 |
| oxidized irgafos 168 | 95906-11-9 | 663 | 0,19 |
| d-limonene | 5989-27-5 | 136,13 | 0,19 |
| bis(2-ethylhexyl) sebacate | 122-62-3 | 427 | 0,19 |
| phosphorous acid, tris(2,4-di-tert-butylphenyl)ester | 31570-04-4 | 646,94 | 0,17 |
| naphthalene | 91-20-3 | 128 | 0,17 |
| hydrocarbons | | | 0,17 |
| tpa-eg oligomers ** | | | 0,14 |
| phthalic acid, bis(2-ethylhexyl) ester | 117-81-7 | 390,6 | 0,14 |
| 3,6,13,16-tetraoxatricyclo[16.2.2.2(8,11)]tetracosa-8,10,18,20,21,23-hexaene-2,7,12,17-tetrone | 1000398-77-0 | 384,09 | 0,14 |
| furfural | 98-01-1 | 96 | 0,13 |
| ethylbenzene | 100-41-4 | 106 | 0,13 |
| ethanol | 64-17-5 | 46,07 | 0,13 |
| cyclic[tpa+deg]2 | | 479,46 | 0,13 |
| cyclic[tpa+eg]2+[ipa+eg] | | 598,11 | 0,13 |
| cyclic[tpa+eg]2+[ipa+deg] | | 634,81 | 0,13 |
| cyclic[tpa+eg]+[ipa+eg] | | 384,08 | 0,13 |

## ANNEX IVb: substances in output for technology configuration Y1Y2

| substance | cas_nr | mw | occurence_ in output/100 |
|---|---|---|---|
| cyclic[tpa+eg]3+[ipa+eg] | | 768,17 | 0,12 |
| cyclic[tpa+eg]+[tpa+deg]2 | | 686,16 | 0,12 |
| cyclic[tpa+eg]+[ipa+deg] | | 428,11 | 0,12 |
| 4(1h)-quinazolinone | 491-36-1 | 146,05 | 0,12 |
| linear[tpa+eg]2+deg | | 512,13 | 0,11 |
| 1-hydroxy-4-(p-toluidino)anthraquinone | 81-48-1 | 329,11 | 0,11 |
| phenol | 108-95-2 | 94,11 | 0,10 |
| oleamide | 301-02-0 | 281,5 | 0,10 |
| nonanal | 124-19-6 | 142 | 0,10 |
| linear[tpa+eg]2+eg | | 468,1 | 0,10 |
| cyclopentanone | 120-92-3 | 84 | 0,10 |
| cyclic[tpa+eg]3+[ipa+deg] | | 480,31 | 0,10 |
| 1,2-ethanediol diformate | 629-15-2 | 118 | 0,10 |
| hexanal | 66-25-1 | 100 | 0,09 |
| cyclic[tpa+eg]4+[ipa+eg] | | 960,21 | 0,09 |
| benzoic acid | 65-85-0 | 122,12 | 0,09 |
| 2-ethyl-1-hexanol | 104-76-7 | 130 | 0,09 |
| octadecanoic acid, 2,3-bis(acetyloxy)propyl ester | 33599-07-4 | 442,33 | 0,09 |
| linear[tpa+eg]2 | | 402,1 | 0,09 |
| erucamide | 112-84-5 | 337,59 | 0,09 |
| cyclic[tpa+eg]4+[tpa+deg] | | 1.026,22 | 0,09 |
| 1,2-ethanediol, monobenzoate | 94-33-7 | 166,06 | 0,09 |
| palmitic acid | 57-10-3 | 256,43 | 0,08 |
| linear[tpa+eg]3+deg | | 380,29 | 0,08 |
| 2,6-dimethyl-pyridine | 108-48-5 | 107 | 0,08 |
| 1-stearoylglycerol (1-monostearin) | 123-94-4 | 380,29 | 0,08 |
| methacrylic acid, methyl ester | 80-62-6 | 100,12 | 0,07 |
| 9-octadecenoic acid (z)-, 2,3-bis(acetyloxy)propyl ester | 55401-64-4 | | 0,07 |
| isophthalaldehyde | 626-19-7 | 134,04 | 0,07 |
| bis(3,4-dimethylbenzylidene)sorbitol | 135861-56-2 | | 0,07 |
| acetic acid, methyl ester | 79-20-9 | | 0,07 |
| 1-butanol | 71-36-3 | 74,12 | 0,07 |
| 1,4-benzenedicarboxaldehyde | 623-27-8 | 134 | 0,07 |
| tri-n-butyl acetyl citrate | 77-90-7 | | 0,06 |
| stearic acid | 57-11-4 | 284,49 | 0,06 |
| pentanal | 110-62-3 | | 0,06 |
| nonylphenol ethoxylates (npeo5) | | 459,29 | 0,06 |
| linear[tpa+eg]3 | | 594,14 | 0,06 |
| heptanal | 111-71-7 | | 0,06 |
| decanal | 112-31-2 | | 0,06 |
| carboxylic acid | | | 0,06 |
| 4(1h)-quinazolinone, 2-methyl- | 1769-24-0 | 160,06 | 0,06 |
| solvent blue 104 | 116-75-6 | 474,23 | 0,06 |
| linear[tpa+eg]3+eg | | 660,15 | 0,06 |
| isopropyl myristate | 110-27-0 | 270 | 0,06 |
| hexamethyl cyclotrisiloxane | 541-05-9 | | 0,06 |
| furan | 110-00-9 | | 0,06 |
| dimethylsilanediol | 1066-42-8 | | 0,06 |
| aldehydes c6-c10 | | | 0,06 |
| 2-propenal | 107-02-8 | | 0,06 |
| 2-butenal | 4170-30-3 | | 0,06 |
| 1-propene-1,2,3-tricarboxylic acid, tributyl ester | 7568-58-3 | | 0,06 |
| 1-hexadecanol | 36653-82-4 | 242,45 | 0,06 |
| α-methylstyrene | 98-83-9 | | 0,05 |
| thiodipropionic acid, didodecyl ester | 123-28-4 | 514,86 | 0,05 |

## ANNEX IVb: substances in output for technology configuration Y1Y2

| substance | cas_nr | mw | occurence_ in output/100 |
|---|---|---|---|
| phenol, 2,4-bis(1-methyl-1-phenylethyl)- | 2772-45-4 | 330,2 | 0,05 |
| pet cyclic trimer | 7441-32-9 | 576,13 | 0,05 |
| octadecanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester | 55401-62-2 | | 0,05 |
| linear[tpa+eg]+deg | | 320,09 | 0,05 |
| citric acid, triethyl ester | 77-93-0 | | 0,05 |
| 4-formyl-benzonitrile | 105-07-7 | 131 | 0,05 |
| 2-pentanone | 107-87-9 | | 0,05 |
| 2,5-bis(5-tert-butyl-2-benzoxazolyl)thiophene | 7128-64-5 | 430 | 0,05 |
| 2,4-di-tert-butylphenol | 96-76-4 | | 0,05 |
| 1,3-dioxolane | 646-06-0 | 74,08 | 0,05 |
| solvent green 3 | 128-80-3 | 418,5 | 0,04 |
| pet cyclic dimer | 24388-68-9 | 384,08 | 0,04 |
| palmitamide | 629-54-9 | 255,44 | 0,04 |
| methyl formate | 107-31-3 | | 0,04 |
| ketones c5-c11 | | | 0,04 |
| isophthalic acid | 121-91-5 | | 0,04 |
| heptane | 142-82-5 | 100 | 0,04 |
| dioctyl adipate | 123-79-5 | 370,31 | 0,04 |
| dihydro-5-methyl-2(3h)-furanone | 108-29-2 | 100 | 0,04 |
| cyclopentasiloxane, decamethyl- | 541-02-6 | 370,09 | 0,04 |
| c[eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | | | 0,04 |
| c[eg/pa/eg/pa/eg/pa] pa=phthalic acid eg=ethylene glycol | | | 0,04 |
| c[eg/pa/eg/pa/eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | | | 0,04 |
| c[eg/pa/eg/pa/eg/pa/eg/pa/eg/pa] eg=ethylene glycol pa=phthalic acid | | | 0,04 |
| c[deg/pa/eg/pa/eg/pa/eg/pa] pa=phthalic acid eg=ethylene glycol deg=diethylene glycol | | | 0,04 |
| c[deg/pa/deg/pa] deg= diethylen glycol pa= phthalic acid | | | 0,04 |
| benzonitrile, 2-amino- | 1885-29-6 | 118,05 | 0,04 |
| benzoic acid, 4-methyl-, 2-hydroxyethyl ester | 28129-15-9 | 180,08 | 0,04 |
| aldehydes c5-c11 | | 44 | 0,04 |
| 2-hexanone | 591-78-6 | | 0,04 |
| 2,4-dimethylfuran | 3710-43-8 | 96 | 0,04 |
| triphenylphosphine oxide | 791-28-6 | 278,09 | 0,04 |
| tetrahydrofuran | 109-99-9 | 72,11 | 0,04 |
| stearamide | 124-26-5 | 283,5 | 0,04 |
| hexanoic acid | 142-62-1 | 116 | 0,04 |
| hexacosane | 630-01-3 | 366,4 | 0,04 |
| ethylene terephthalate cyclic tetramer | 16104-96-4 | 768,67 | 0,04 |
| ethylene carbonate | 96-49-1 | 88,06 | 0,04 |
| dodecane | 112-40-3 | 170 | 0,04 |
| cyclotetrasiloxane, octamethyl- | 556-67-2 | 296,08 | 0,04 |
| c[deg/pa/eg/pa] pa=phthalic acid deg=diethylen glycol eg=ethylen glycol | | 428,11 | 0,04 |
| c[deg/pa/eg/pa/eg/pa] pa=phthalic acid deg=diethylen glycol eg=ethylen glycol | | 620,15 | 0,04 |
| bis-gma / bisphenol a glycidylmethacrylate | 1565-94-2 | 843,24 | 0,04 |
| aldehydes c6-c12 | | | 0,04 |
| 2-propanol | 67-63-0 | 60,1 | 0,04 |
| 2-heptanone | 110-43-0 | | 0,04 |
| 2,2'-(1,4-phenylene)bis[4H-3,1-benzoxazin-4-one] | 18600-59-4 | 369 | 0,04 |
| 1-decanol, 2-hexyl- | 2425-77-6 | | 0,04 |
| 1-acetoxyacetone | 592-20-1 | 116 | 0,04 |
| unknown substance [m/z: 341.0, 208.0, 236.0] | | 0 | 0,03 |
| succinic anhydride | 108-30-5 | 100 | 0,03 |
| p-toluic acid, 5-tridecyl ester | | 318,3 | 0,03 |
| probable pet oligomer (dimer ether) | | | 0,03 |
| probable pet oligomer (cyclic dimer) | | | 0,03 |
| polyethyleneglycol (eo = 1-50) ethers of linear and branched primary (c 8-c 22) alcohols | | | 0,03 |

| ANNEX IVb: substances in output for technology configuration Y1Y2 | | | |
|---|---|---|---|
| **substance** | **cas_nr** | **mw** | **occurence_ in output/100** |
| p-cymene | 99-87-6 | 134 | 0,03 |
| octanal + d-limonene | 124-13-0 + 5989-27-5 | | 0,03 |
| octadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 621-61-4 | 358,3 | 0,03 |
| n-butylbenzenesulphonamide (n-butylbenzenesulfonamide) | 3622-84-2 | 213,08 | 0,03 |
| myristic acid | 544-63-8 | 228,38 | 0,03 |
| methyl hydroxyacetate | 96-35-5 | | 0,03 |
| l[eg/pa/eg/pa/eg] eg=ethylen glycol pa=phthalic acid | | | 0,03 |
| ketones c5-c8 | | | 0,03 |
| hexyl 2-(1-hexoxy-1-oxopropan-2-yl)sulfanylpropanoate | | 346,22 | 0,03 |
| hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 23470-00-0 | 330,28 | 0,03 |
| heptane, 2,2,4,6,6-pentamethyl- | 13475-82-6 | 170 | 0,03 |
| eucalyptol | 470-82-6 | 154 | 0,03 |
| ethylene (tere-,iso-)phthalate cyclic pentamer_pto | 16104-97-5 | 960,21 | 0,03 |
| ethoxylated bisphenol a diacrylate | 64401-02-1 | 446,17 | 0,03 |
| eicosanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester | 55429-68-0 | | 0,03 |
| cyclohexasiloxane, dodecamethyl- | 540-97-6 | 444,11 | 0,03 |
| carboxylic acids | | | 0,03 |
| carbonic acid, eicosyl vinyl ester | 1000382-54-3 | 368 | 0,03 |
| caprylic acid | 124-07-2 | 144,22 | 0,03 |
| caprolactone | 502-44-3 | | 0,03 |
| butyraldehyde | 123-72-8 | 72,11 | 0,03 |
| aldehydes c6-c9 | | | 0,03 |
| acrylic acid, dodecyl ester | 2156-97-0 | | 0,03 |
| 3,3'-dimetoxy-benzidin | 119-90-4 | 408,29 | 0,03 |
| 2-octanone | 111-13-7 | | 0,03 |
| 2-ethylhexyl-acetate | 103-09-3 | 172 | 0,03 |
| 2-butanone | 78-93-3 | | 0,03 |
| (m-z : 193.0-149.0-104.0-175.0); possible linear oligomer: terephathalic acid - ethylene glycol | | | 0,03 |
| (m-z : 130.0-117.0-371.3-239.2) | | | 0,03 |

# Annex V: Most occurring substances

ANNEX V: Most occuring substances

| | substances in the input | cas_nr | mol weight | occurrence in input/100 | position in Reg. (EU) 10/2011 | X1X2W variation input/output % | Y1Y2 variation input/output % |
|---|---|---|---|---|---|---|---|
| 1 | 2-methyl-1,3-dioxolane | 497-26-7 | 88,0 | 0,95 | NIAS- covered by Art. 6(4) | -50,5 | -40,1 |
| 2 | acetaldehyde | 75-07-0 | 44,1 | 0,80 | authorized without SML | 31,6 | 70,1 |
| 3 | benzene | 71-43-2 | 78,0 | 0,78 | NIAS- covered by Art. 6(4) | 126,4 | 529,6 |
| 4 | acetic acid | 64-19-7 | 60,1 | 0,69 | authorized without SML | 89,6 | -26,1 |
| 5 | benzaldehyde | 100-52-7 | 106,0 | 0,64 | authorized without SML | -67,1 | -77,7 |
| 6 | formic acid | 64-18-6 | 46,0 | 0,61 | authorized without SML | 74,7 | -16,1 |
| 7 | acetic acid, ethyl ester | 141-78-6 | 88,1 | 0,60 | authorized without SML | -55,3 | -72,2 |
| 8 | pet oligomers | n.a | n.a | 0,59 | Covered by the general safety requirements of Art. 3 | | |
| 9 | terephthalic acid | 100-21-0 | 166,1 | 0,58 | authorized with SML = 7.5 mg/kg (group restriction ) | 33,3 | 29,9 |
| 10 | acetone | 67-64-1 | 58,0 | 0,57 | authorized without SML | 229,9 | -56,0 |
| | ethyleneglycol | 107-21-1 | 62,1 | 0,57 | authorized with SML = 30 mg/kg (group restriction ) | -44,8 | 2,8 |
| | ethanol | 64-17-5 | 46,1 | 0,57 | authorized without SML | -98,5 | -92,3 |
| 11 | limonene | 138-86-3 | 136,0 | 0,54 | NIAS- covered by Art. 6(4) | -94,6 | -86,6 |
| | toluene | 108-88-3 | 92,0 | 0,54 | NIAS- covered by Art. 6(4) | -88,4 | -91,0 |
| 12 | acetophenone | 98-86-2 | 120,0 | 0,52 | NIAS- covered by Art. 6(4) | -73,3 | -62,9 |
| | 2-pentyl-furan | 3777-69-3 | 138,0 | 0,52 | NIAS- covered by Art. 6(4) | -76,5 | -60,2 |
| 13 | butyrolactone | 96-48-0 | 86,0 | 0,49 | NIAS- covered by Art. 6(4) | 79,9 | 23,7 |
| 14 | tpa-eg oligomers | n.a | n.a | 0,45 | Covered by the general safety requirements of Art. 3 | | |
| 15 | phosphorous acid, tris(2,4-di-tert-butylphenyl)ester | 31570-04-4 | 646,9 | 0,40 | authorized without SML | -54,0 | -81,9 |
| | aibn | 78-67-1 | 164,0 | 0,40 | NIAS- covered by Art. 6(4) | -83,8 | -88,5 |
| | oleamide | 301-02-0 | 281,5 | 0,40 | authorized without SML | -99,6 | -86,9 |
| 16 | xylenes | n.a | 106,0 | 0,39 | NIAS- covered by Art. 6(4) | -95,3 | -82,5 |
| | styrene | 100-42-5 | 104,2 | 0,39 | authorized without SML | -30,0 | -33,0 |
| 17 | oxidized irgafos 168 | 95906-11-9 | 663,0 | 0,37 | NIAS- covered by Art. 6(4) | -7,1 | -53,5 |
| | 2,2-bis(4-hydroxyphenyl)propane (BPA) | 80-05-7 | 228,3 | 0,37 | The intentional use of BPA in food contact materials will be prohibited by a forthcoming Regulation that will amend Reg. 10/2011. | -20,6 | 22,3 |
| | 2-[2-hydroxy-3,5-bis(1,1-dimethylbenzyl)phenyl]benzotriazole | 70321-86-7 | 447,0 | 0,37 | authorized with SML = 1.5 mg/kg | 269,2 | -8,8 |
| 18 | 2-ethyl-1-hexanol | 104-76-7 | 130,0 | 0,34 | authorized with SML = 30 mg/kg | -98,2 | -97,8 |
| 19 | 1,4-benzenedicarboxylic acid, bis(2-hydroxyethyl) ester (BHET) | 959-26-2 | 254,1 | 0,33 | NIAS- covered by Art. 6(4) | -23,3 | 1,9 |
| 20 | bis(2-ethylhexyl) sebacate | 122-62-3 | 427,0 | 0,30 | NIAS- covered by Art. 6(4) | -86,8 | -95,6 |
| | 1,2-ethanediol, monoacetate | 542-59-6 | 104,0 | 0,30 | NIAS- covered by Art. 6(4) | -35,1 | -23,4 |
| | aldehydes | n.a | | 0,30 | Depending on the specific chemical formula, they can be covered by Art. 6(49 as NIAS | -12,9 | -63,4 |
| 21 | ketones | n.a | | 0,29 | Depending on the specific chemical formula, they can be covered by Art. 6(49 as NIAS | 141,1 | -87,7 |
| 22 | 1-pentanol | 71-41-0 | 88,2 | 0,28 | authorized without SML | 109,8 | -22,8 |
| | terephthalic acid, bis(2-ethylhexyl)ester | 6422-86-2 | 390,6 | 0,22 | authorized with SML = 60 mg/kg (group restriction ) | -22,3 | -79,0 |
| | phthalic acid, bis(2-ethylhexyl) ester | 117-81-7 | 390,6 | 0,17 | authorized with SML = 0.6 mg/kg (group restriction )- Only to be used as: (a) plasticiser in repeated use materials and articles contacting non-fatty foods; (b) technical support agent in concentrations up to 0,1 % (w/w) in the final product. | -93,3 | -69,7 |

# Annex VI: Summary of testing methods

Testing laboratories and relevant methods of analysis for volatile substances

| VOLATILE SUBSTANCES | Data | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Laboratory** | **Company** | **LAB 1** | **LAB 2** | **LAB 3** | **LAB 4** | **LAB 5** | **LAB 6** | **LAB 7** | **LAB 8** | **LAB 9** |
| **Sample** | Date of Arrival | 06/03/2024 | 08/03/24 | 11/03/2024 | 06/03/2024 | 06/03/2024 | 06/03/2024 | 14/03/2024 | 06/03/2024 | 20/03/2024 |
| **Grinding** | Make | Biometa tecnologia y sistemas S.A. | Retsch | / | SPEX | cryogenic mill | IKA | IKA | Retsch | RETSCH |
| | Model | ZM2000 | ZM300 | / | 6875 freezer/mill | CryoMill Retsch | A 11 B S000 | A 11 B S000 | ZM 200 | ZM200 Ultra Centrifugal Mill 0.5 mm |
| | Temp (ºT) | -200 | maximum 20 | / | ≈-196 | - 196 | -196 | -196 | Before grinding, sample cooled to: -196 | -196 |
| | Coolant | Nitrogen | dry ice | / | Liquid nitrogen | liquid nitrogen | Liquid Nitrogen | Liquid Nitrogen | Liquid Nitrogen | Liquid nitrogen |
| **Instrument** | Chromatograph Model | Thermo Fisher Scientific | GC 8890 | QP2010 | 7890B | 7890A Agilent | 7890B | 8890-G3542A | 7890B | GC 8860 |
| | Chromatograph Make | - | Agilent | Shimadzu | Agilent | Agilent | Agilent | Agilent | Agilent Technologies | Agilent |
| | Detector1 Model | Thermo Fisher Scientific | 5977B | QP2010 | FID | GC 7000 MS Triple Quad | 5977B | 5977B-G7081B | 5977B | MS 5977B |
| | Detector1 Make | - | Agilent | Shimadzu | Agilent | Agilent | Agilent | Agilent | Agilent Technologies | Agilent |
| | Detector2 Model | | \ | | 0 | GC 7000 MS Triple Quad | | | - | |
| | Detector2 Make | | \ | | 0 | Agilent | | | - | |
| | Chromatographic Column | (5%-phenyl)-methylpolysiloxane | DB 624 | J&W DB-624 Ultra Inert GC Column, 30 m, 0.25 mm, 1.40 µm, | DB-1, 30m x 0.25 mm x 0.25 µm | DB624 Agilent | Restek Rtx-5MS | VF-624ms (30 m, 0.25 mm, 1.40 µm) | Restek Rtx-200 | HP-5 MS 30 m x 0.25 mm x 0.25 µm |
| | Extraction Technique | Thermal desorption | thermal desorption in headspace vial | HS | Multi-headspace extraction | SPME | HS | Head space | Dynamic headspace | HS-SPME |
| | Extraction Time (h) | 1 | 1 | 1 | 3 | 0.5 | 1 | 1 | 1 | 0.33 |
| | Extraction Temperature (ºC) | 100 | 200 | 120 | 90 | 65 | 200 | 200 | 150 | 120 |
| **Test Conditions** | Range of Mass Acquisition | 20-400 | 35-450 | 29-300 | 0 | 30-600 mz | 41-400 | 25-400 | 33-550 | 45-450 |
| | Internal Standard | Toluene | Styrene Deuterated D8 | Pentyl benzene | 0 | Benzene - d 6 | Mix of volatiles | Chlorobenzene (CAS No. 108-90-7) | Styrene-d8 | NO |
| **Performances** | Sensitivity1 | 150 | 30 µg/kg | 30 ug/kg | 0 | 0.01 | 30 µg/kg | 50 | 10 ppb | not specified |
| **Identification of Compounds** | Library | NIST | VOCsMXNSC (internal database); NIST11; NIST17, WILEY275 | Nist | 0 | NIST | NIST | NIST17 and Internal Library | NIST17, in-house libraries | NIST 20 |

Testing laboratories and relevant methods of analysis for semi-volatile substances

| SEMI VOLATILE SUBSTANCWS | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Laboratory** | **Company** | **LAB1** | **LAB 2** | **LAB 3** | **LAB 4** | **LAB 5** | **LAB 6** | **LAB 7** | **LAB 8** | **LAB 9** |
| **Sample** | Date of Arrival | 06/03/2024 | 08/03/2024 | 11/03/2024 | 06/03/2024 | 06/03/2024 | 13/03/2024 | 14/03/2024 | 06/03/2024 | 20/03/2024 |
| **Grinding** | Make | Biometa tecnologia y sistemas S.A. | Retsch | / | SPEX | cryogenic mill | IKA | IKA | Retsch | RETSCH |
| | Model | ZM2000 | ZM300 | / | 6875 freezer/mill | CryoMill Retsch | A 11 B S000 | A 11 B S000 | ZM 200 | ZM200 Ultra Centrifugal Mill 0.5 mm |
| | Temp | -200 | maximum 20 | / | ≈-196 | - 196 | -196 | -196 | Before grinding, sample cooled to: -196 | -196 |
| | Coolant | Nitrogen | dry ice | / | Liquid nitrogen | liquid nitrogen | Liquid Nitrogen | Liquid Nitrogen | Liquid Nitrogen | Liquid nitrogen |
| **Instrument** | Chromatograph Model | Thermo Fisher Scientific | 7890B | GC8890 | G3540A | 7890A Agilent | GC-MS | 7890A | 6890N | GC 8860 |
| | Chromatograph Make | - | Agilent | Agilent | Agilent | Agilent | Agilent | Agilent | Agilent Technologies | Agilent |
| | Detector1 Model | Thermo Fisher Scientific | G7039A | TQ7000E | 5977B GC/MSD | GTC premier Tof Waters | G3440A | G3171A | 5975C | MS 5977B |
| | Detector1 Make | - | Agilent | Agilent | Agilent | Waters | Agilent | Agilent | Agilent Technologies | Agilent |
| | Detector2 Model | | \ | | FID | GTC premier Tof Waters | ND | | - | |
| | Detector2 Make | | \ | | Agilent | Waters | ND | | - | |
| | Chromatographic Column | (5%-phenyl)-methylpolysiloxane | DB-5ms | Column DB-5 30m, 0.25mm, 0.25µm | OPTIMA DELTA-3 ID: 30 m x 0,32 mm x,0,25 µm | HP5-MS | Rxi-1HT | HP-5MS UI (30 m, 0.25 mm, 0.25 µm) | Restek Rxi-5Sil MS | HP-5 MS 30 m x 0.25 mm x 0.25 µm |
| **Extraction Conditions** | Extraction Solvent | Hexane/Ethanol 3:1 | Dichloromethane | Dichloromethane | Dichloromethane | Dichloromethane and Acetonitrile | Dichloromethane | Acetonitrile | Dichloromethane | not applicable (HS-SPME) |
| | Type of Contact | Immersion | immersion | / | Solid-liquid extraction | Soxhlet | ultrasonic bath | Total immersion | Liquid extraction by shaking | HS-SPME |
| | Sample Weight (gr) | 1.5 | 1 | 2 | 1 | 15 | 0.3 | 1 | 5 | 1,2 |
| | Solvent Volume (ml) | 15 | 15 | 10 | 15 | 250 | 5 | 10 | 50 | 0 |
| | Time of Contact (h) | 8 | 8 | 2 | 24 | 24 | 6 | 1 | 1 | 0,33 |
| | Temperature of Contact (°T) | 20 | 70 | 60 | 40 | 100 | 60 | 60 | 30 | 120 |
| **Test Conditions** | Range Of Mass Acquisition | 25-300 | 35÷1000 | 30-550 | 30-800 | 60-800 mz | 33-750 amu | 45-700 | 33-550 | 45-450 |
| | Internal Standard | - | 4,4-difluorobiphenyl | d5-Chlorobenzene,B21-BHT,D10-fenantrene | MOSH/MOAH Standard 150-600 µg/mL | Benzofenone | Methyl Heptadecanoate | Dipropyl phthalate (CAS No. 131-16-8) | Phenol-d5, n-Butylphthalimide, 1-Fluoronaphthalene | NO |
| | Quantification | Toluene | \ | / | semi quantitative via FID | N/A | ND | Semi-quantification | Semi-quantification using an internal standard | not specified |
| **Performances** | Sensitivity1 | 100 | 100 µg/Kg | 0,1 | autotune | 0.01 | 200 | 1000 | 10 ppb | not specified |
| **Identification of Compounds** | Library | NIST | SVOCsMXNSC (internal database); NIST11; NIST17, WILEY275 | NIST v2,4 25 March 2020 | NIST | NIST | ND | NIST17 and Internal library | NIST17, in-house libraries | NIST 20 |

Testing laboratories and relevant methods of analysis for non-volatile substances

| NON_VOLATILE SUBSTANCES | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Laboratory** | **Company** | **LAB1** | **LAB 2** | **LAB 3** | **LAB 4** | **LAB 5** | **LAB 6** | **LAB 7** | **LAB 8** | **LAB 9** |
| **Sample** | Date of Arrival | 06/03/2024 | 08/03/2024 | 11/03/2024 | 06.03.2024 | 06/03/2024 | 13/03/2024 | 14/03/2024 | 06/03/2024 | 20/03/2024 |
| | Client Sample Reference Number | Sheet 2 | Sheet 1 | Sheet 2 | Sheet 2 | Sheet 2 | Sheet 2 | Sheet 1 | Sheet 2 | Sheet 2 |
| | Laboratory Sample Reference Number | 24-1082-2 | 24.509868_1-2-3 | QC240005.01 | 141102-3/24/TYC | Reference 2 | 216-OU-24 | 24LD00844 | Reference 2 | Reference 2 |
| | Date of Analysis Start | 11/03/2024 | 08/03/2024 | 13/03/2024 | 26.03.2024 | 07/03/2024 | 18/03/2024 | 20/03/2024 | 08/03/2024 | 21/03/2024 |
| | Date of Report | 09/04/2024 | 22/04/2024 | 05/04/2024 | 30.03.2024 | 05/04/2024 | 18/03/2024 | 04/04/2024 | 26/03/2024 | 27/03/2024 |
| **Grinding** | Make | Biometa tecnologia y sistemas S.A. | Retsch | / | SPEX | cryogenic mill | IKA | Retsch | Retsch | RETSCH |
| | Model | ZM2000 | ZM300 | / | 6875 freezer/mill | CryoMill Retsch | A 11 B S000 | ZM200 | ZM 200 | ZM200 Ultra Centrifugal Mill 0.5 mm |
| | Temp | -200 | maximum 20 | / | ≈-196 | - 196 | -196 | -196 | Before grinding, sample cooled to: -196 | -196 |
| | Coolant | Nitrogen | dry ice | / | Liquid nitrogen | liquid nitrogen | Liquid Nitrogen | liquid nitrogen | Liquid Nitrogen | Liquid nitrogen |
| **Instrument** | Chromatograph Model | Waters | Vanquish | Nexera X2 | 1260 Infinity II | Xevo G2-XS Qtof Waters | HPLC | Nexera X2 | 1290 Infinity II | Acquity Xevo |
| | Chromatograph Make | - | Thermo Fisher | Shimadzu | Agilent | Waters | Shimadzu | SHIMADZU | Agilent | Waters |
| | Detector1 Model | Waters | Orbitrap Exploris 120 | TripleTOF4600 | 6546 LC/Q-TOF | Qtof Waters | LCMS (8045) | TRIPLETOF 4600 | ZenoTOF 7600 | Xevo G2 QTOF |
| | Detector1 Make | - | Thermo Fisher | Sciex | Agilent | Waters | Shimadzu | AB SCIEX | Sciex | Waters |
| | Detector2 Model | - | | | 0 | Xevo G2-XS Qtof Waters | | | 1290 Infinity II DAD | |
| | Detector2 Make | - | | | 0 | Waters | | | Agilent | |
| | Chromatographic Column | C18, 1.6um x 2.1 mm x 100mm | Aquity UPLC HSS T3-C18 | Kinetex EVO C18 150x21 mmm 2,6 um | ACQUITY UPLC BEH C18 Column, 130Å, 1.7 µm, 2.1 mm X 100 mm | ACQUITY UPLC BEH C18 Column, 130Å, 1.7 µm, 2.1 mm X 50 mm, 1/pk | Raptor C18 2.7 µm 100 x 2.1 mm | Kinetex 2.6 µm EVO C18, 50 x 2.1mm | Macherey Nagel NUCLEOSHELL Biphenyl | Acquity UPLC BEH C18 17 µm particle size (2.1 mm x 100 mm) |
| **Extraction Conditions** | Extraction Solvent | Hexane/Etanol 3:1 | Dichloromethane | Acetonitrile | Acetonitrile | Dichloromethane and Acetonitrile | Dichloromethane | Acetonitrile | Acetonitril | 1,1,1,3,3,3-hexafluoroisopropanol (HFIP)/ Methanol |
| | Type of Contact | Immersion | immersion | / | Solid-liquid extraction | Soxhlet extraction | ultrasonic bath | Total immersion | Ultrasonification | Total dissolution |
| | Sample Weight (gr) | 1.5 | 1 | 2 | 1 | 15 | 0.3 | 1 | 1 | 0,4 |
| | Solvent Volume (ml) | 15 | 15 | 10 | 15 | 250 | 5 | 10 | 10 | 4 mL HFIP and 10 mL MeOH |
| | Time of Contact (h) | 8 | 8 | 2 | 24 | 24 | 6 | 1 | 1 | 24 |
| | Temperature of Contact (ºC) | 20 | 70 | 60 | 60 | 100 | 60 | 60 | 70 | 40 |
| **Test Conditions** | Range of Mass Acquisition | 70-1000 | 70÷1000 | 20-1200 | 50-1700 | 50-1200 m/z | 50-750 | 100 - 1600 | 70-1200 | 50-1200 |
| | Polarity | Positive and negative | POS/NEG | pos and neg | ESI+ | ESI + and ESI - | POS AND NEG | Negative | positive and negative | Positive |
| | POS Internal Standard | Benzyl butyl phthalate | Benzyl butyl phthalate-3,4,5,6-d4 | relative compounds | Reserpina, Pyraclostrobin, Acetmiprid | Diallyl phthalate | ND | UV-234 (CAS No. 70321-86-7) | Otylisothiazolinon, Dilauryl thiodipropionate | Leucine Enkephalin |
| | NEG Internal Standard | Nimesulide | Nimesulide | relative compounds | n.a. | Bisphenol A | TPA for oligomers semi-quantification | Taurocholic acid (CAS No. 81-24-3) | Palmitic acid-d31 | not defined |
| **Performances** | Sensitivity1 | 100 | 100 µg/Kg | 100 ug/kg | check tune, on-line references masses | 0.01 | ND | 1000 | 10 ppb | $MS^E$ mode |
| **Identification of Compounds** | **Library** | **Internal** | **NVOCsMXNS-C and NVC** | **Internal library** | **PCDL (in-house library)** | **ITENE** | **-** | **NIST 2017 and Internal** | **Sciex E&L libraries, in-h** | **not defined** |