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Application News

Py-Screener™ Ver. 3: Simultaneously Test for Substances Regulated Under RoHS, TSCA, and POPs

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User Benefits

- In just one analysis, Py-Screener Ver. 3 can determine levels of phthalate esters, brominated flame retardants (PBBs, PBDEs), PIP (3:1), UV-328, dechlorane plus (DP), short-chain chlorinated paraffins (SCCPs), and medium-chain chlorinated paraffins (MCCPs).
- It can also test for SCCPs and MCCPs by electron ionization (EI) instead of negative chemical ionization (NCI).
- PIP (3:1), UV-328, DP, and SCCPs and MCCPs can be screened without the need for corresponding reference materials.

■ Introduction

Countries and regulatory bodies worldwide are introducing increasingly stringent regulations on the chemical substances used in electronic devices and industrial products. The RoHS Directive and REACH regulations in the EU, the Toxic Substances Control Act (TSCA) in the USA, and the Stockholm Convention on Persistent Organic Pollutants (POPs) are also targeting an increasingly broad range of substances. Therefore, manufacturers are required to accurately identify regulated substances in their products and comply with each regulation.

While Py-Screener Ver. 2 can screen for seven phthalate esters and brominated flame retardants, including substances regulated under the RoHS Directive, version 3 can also screen for PIP (3:1), which is regulated under the TSCA, as well as UV-328, DP, and SCCPs and MCCPs , which are regulated under the Stockholm Convention on POPs. A list of supported substances is shown in Table 1.

This article introduces the simultaneous analysis of multiple regulated substances and a case study of testing specific regulated substances in samples, using Py-Screener Ver. 3.

Table 1 Substances that can be Screened

Regulation	Regulated Substances	Version of Py-Screener
RoHS	Phthalate esters (DIBP, DBP, DEHP, and BBP)	Measurable since Py-Screener Ver. 2 and 3
	Brominated flame retardants (PBBs, PBDEs)	
US TSCA	PIP (3:1)	Added for Py-Screener Ver. 3 (specific regulated substances *1)
POPs Convention	UV-328	
	DP	
	SCCPs and MCCPs	

*1 The following are the CAS registry numbers of specific regulated substances: PIP (3:1): 68937-41-7, UV-328: 25973-55-1, DP: 13560-89-9, SCCPs: 85535-84-8, and MCCPs: 85535-85-9

■ Analysis Process

Py-Screener Ver. 3 can determine levels of phthalate esters and brominated flame retardants contained in products in accordance with the international analytical standards IEC62321-8 and IEC62321-3-3. It can also test for specific regulated substances (Table 1) under the same conditions and in the same analysis.

In this test, background intensity and instrument sensitivity (S/N) were verified before analyzing samples. These parameters are prescribed by IEC62321-8 to ensure the accuracy of the methods used. Background intensity and instrument sensitivity were determined using a reference material (PN: 225-31003-91)*1 that consisted of a plastic sheet that was spiked with seven phthalate esters. The results met the criteria for both parameters.

*1 Includes three reference materials: blank (for background measurement), 100 mg/kg (to check sensitivity), and 1000 mg/kg (to prepare a calibration curve).

The testing workflow is shown in Fig. 1. Before testing samples, calibration curves were prepared by analyzing the 1000 mg/kg phthalate ester reference material and polypropylene spiked with brominated flame retardants (ERM-EC591). A hole puncher was used to punch out two discs at a time of the phthalate ester reference material, and a cutter was used to obtain pieces of the other materials. Each material was weighed in a sample cup for analysis. During the analysis of samples, phthalate esters and some of the regulated brominated flame retardants were quantitated using a one-point calibration curve. The remaining brominated flame retardants and specific regulated substances were quantitated using the correction factor database*2 that is included with Py-Screener Ver. 3.

*2 Details of the correction factor database can be found in the Py-Screener Ver. 3 catalog.

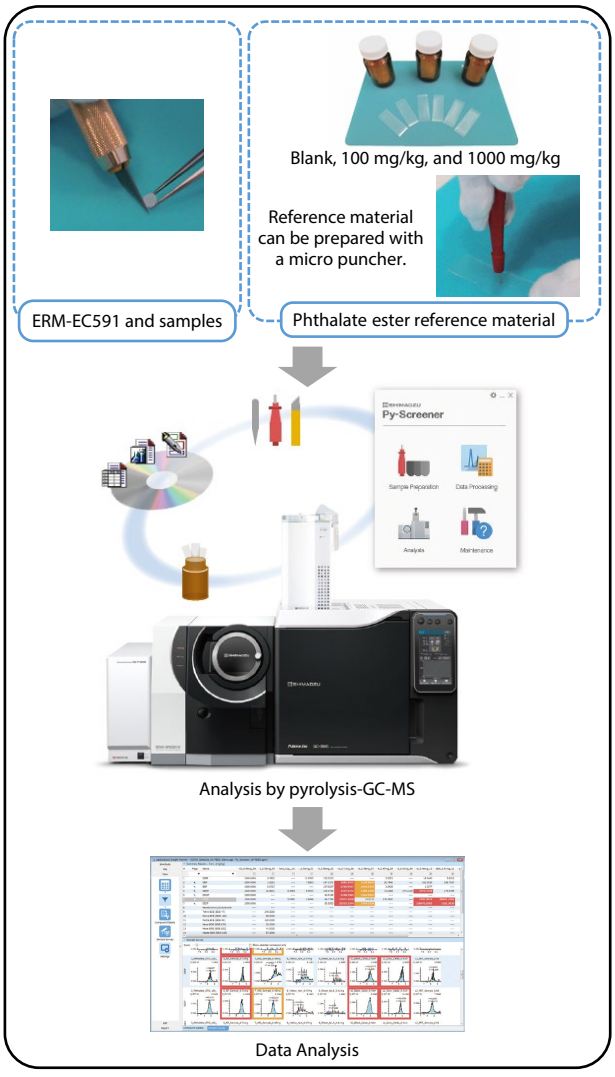


Fig. 1 Testing Workflow

■ Results of Simultaneous Analysis

Fig. 2 shows the results of phthalate esters, brominated flame retardants, and specific regulated substances that were obtained from just a single analysis. Table 2 shows each compound, its relevant grouping, and the corresponding quantifier ion used in SIM mode. The analysis was performed under the conditions shown in Table 3.

SCCPs and MCCPs include many different isomers and require a highly selective analytical technique for quantitation. Negative chemical ionization (NCI) is a widely used approach, while Py-Screener Ver. 3 employs electron ionization (EI), enabling simultaneous analysis of these compounds along with other regulated substances.

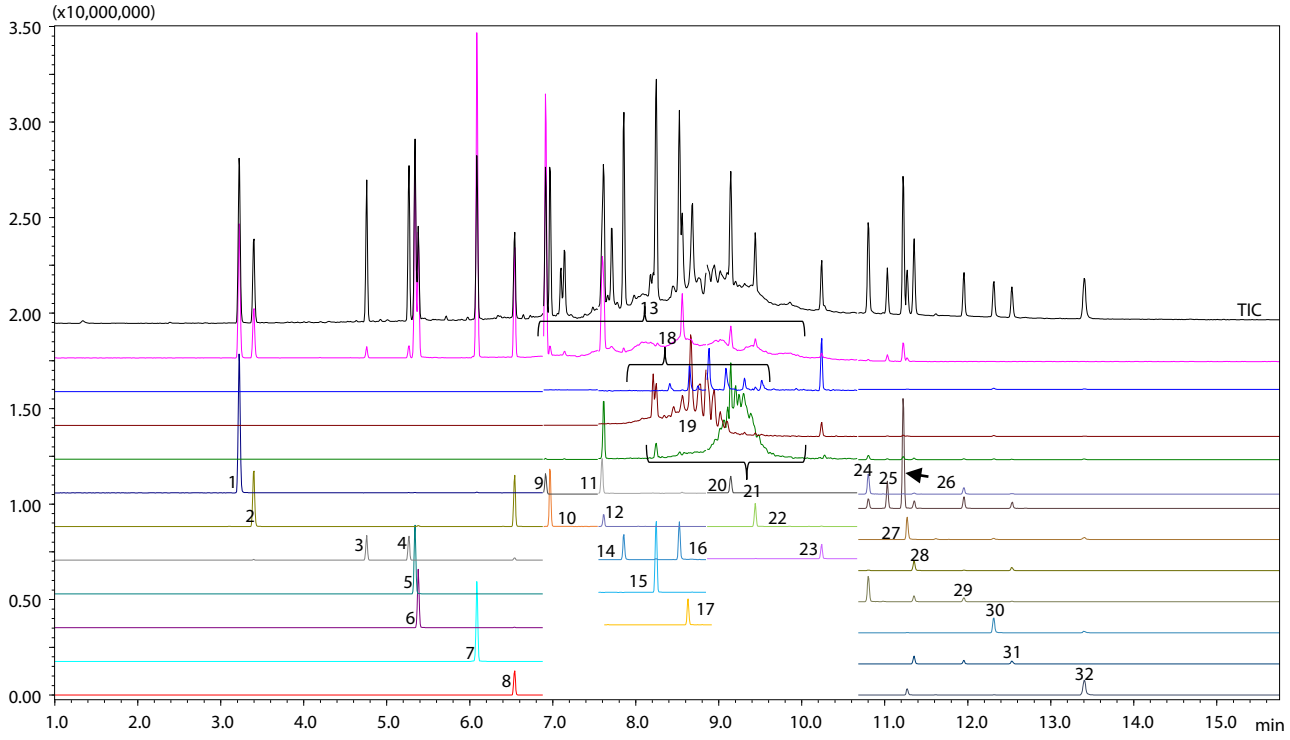


Fig. 2 Results from Simultaneous Analysis for Phthalate Esters, Brominated Flame Retardants, PIP (3:1), UV-328, DP, and SCCPs/MCCPs*1

1 Mono-BB	5 Di-BB	9 Tetra-BB	13 SCCPs+MCCPs	17 Penta-BDE	21 DIDP	25 Syn-Dechlorane Plus	29 Nona-BB
2 Mono-BDE	6 Di-BDE	10 BBP	14 DEHP	18 PIP(3:1)	22 Hexa-BDE	26 Anti-Dechlorane Plus	30 Nona-BDE
3 DIBP	7 Tri-BB	11 Tetra-BDE	15 UV-328	19 DINP	23 Hepta-BDE	27 Octa-BDE	31 Deca-BB
4 DBP	8 Tri-BDE	12 Penta-BB	16 DNOP	20 Hexa-BB	24 Hepta-BB	28 Octa-BB	32 Deca-BDE

Table 2 Compound Information

No.	Compound Name	Grouping	Quantifier Ion (*m/z*)
1	Mono-BB	PBBs	233.9
2	Mono-BDE	PBDEs	247.9
3	DIBP	Phthalate Esters	223.0
4	DBP	Phthalate Esters	223.0
5	Di-BB	PBBs	313.8
6	Di-BDE	PBDEs	327.8
7	Tri-BB	PBBs	389.8
8	Tri-BDE	PBDEs	405.8
9	Tetra-BB	PBBs	467.6
10	BBP	Phthalate Esters	206.0
11	Tetra-BDE	PBDEs	325.8
12	Penta-BB	PBBs	545.6
13	SCCPs+MCCPs*1	CP	49.0
14	DEHP	Phthalate Esters	279.0
15	UV-328	UV	322.2
16	DNOP	Phthalate Esters	279.0
17	Penta-BDE	PBDEs	403.8
18	PIP(3:1)	PIP	452.2
19	DINP	Phthalate Esters	293.0
20	Hexa-BB	PBBs	467.6
21	DIDP	Phthalate Esters	307.0
22	Hexa-BDE	PBDEs	483.6
23	Hepta-BDE	PBDEs	561.6
24	Hepta-BB	PBBs	545.6
25	Syn-Dechlorane Plus	DP	271.8
26	Anti-Dechlorane Plus	DP	271.8
27	Octa-BDE	PBDEs	641.5
28	Octa-BB	PBBs	625.5
29	Nona-BB	PBBs	703.4
30	Nona-BDE	PBDEs	719.4
31	Deca-BB	PBBs	783.3
32	Deca-BDE	PBDEs	799.3

*1 SIM chromatograms show the quantifier ion that corresponds to each compound. For SCCPs and MCCPs, the SIM chromatogram shows the *m/z* 75 qualifier ion.

Table 3 Analysis Conditions

Equipment		
Pyrolyzer Unit	:	EGA/PY-3030D Multi-Shot Pyrolyzer AS-2020E Auto-Shot Sampler (Frontier Laboratories Ltd.)
GC-MS	:	GCMS-QP2020 NX
Py-GC-MS		
[Py]		
Analysis Mode	:	Heart-Cut EGA
Thermal Desorption Temp.	:	200 °C - 20 °C/min - 300 °C - 5 °C/min - 340 °C (1 min)
ITF Temp.	:	300 °C (Manual)
[GC]		
Column	:	SH-1MS (15 m*2 × 0.25 mm I.D., df = 0.1 µm) *3
Oven Temp.	:	80 °C (0 min) - 20 °C/min - 320 °C (4 min)
Sample Vaporization Chamber	:	300 °C
Carrier Gas	:	He
Control Mode	:	Constant linear velocity (52.1 cm/s)
Injection Method	:	Split
Split Ratio	:	50
[MS]		
ITF Temp.	:	320 °C
Ion Source Temp.	:	230 °C
Ionization Method	:	EI
Measurement Mode	:	FASST (simultaneous Scan/SIM measurements)
Scan Mass Range:	:	*m/z* 50-1000
Scan Event Time:	:	0.15 sec
Scan Speed:	:	10000 u/sec
SIM Event Time:	:	0.30 sec
SIM Micro-Scan Width:	:	0.3 u

*2 Separation column (15 m) and guard column (2 m)

*3 PN: 227-36346-01

■ Sample Test Results

Calibration curves were prepared from the 1000 mg/kg phthalate ester reference material and the polypropylene spiked with brominated flame retardants (ERM-EC591).

The samples were capacitor plastic, a PVC sample, an ABS sample, and an insulator cord. Fig. 3 shows the analysis schedule list (Batch Table) as it appears in the GCMS system analysis software (GCMSsolution™). The batch table can be populated with sample amounts, allowing the software to automatically adjust the calibration curve and calculate the correct sample concentration even when different amounts of reference material and samples are used.

	Vial#	Sample Name	Sample Amt.	Sample ID	Sample Type
1	1	Blank_Cup	0.5		0:Unknown
2	2	Phthalate_STD_Blank	0.54		0:Unknown
3	3	Phthalate_STD_100	0.56		2:Control
4	4	Phthalate_STD_1000	0.62		1:Standard:(1)
5	5	ERM-EC591	0.53		1:Standard
6	6	Capacitor Plastic	0.55		0:Unknown
7	7	PVC Sample	0.45		0:Unknown
8	8	ABS Sample	0.52		0:Unknown
9	9	Insulator Cord	0.46		0:Unknown

Fig. 3 Example Batch Table from GCMSsolution

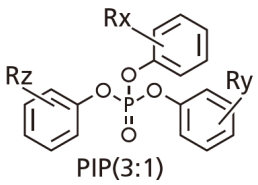
The concentrations of specific regulated substances measured in the samples are shown in Table 4. They were calculated using relative correction factors linked to DEHP. SIM chromatograms of the specific regulated substances are shown in Figs. 5 to 7 and Fig. 10.

Table 4 Quantitative Results for Samples

No.	Compound Name	Sample Concentration (mg/kg)			
		Capacitor Plastic	PVC Sample	ABS Sample	Insulator Cord
1	PIP (3:1)	1344	698	N.D.	N.D.
2	UV-328	N.D.	71	N.D.	N.D.
3	Syn-DP	N.D.	N.D.	112	N.D.
4	Anti-DP	N.D.	N.D.	347	N.D.
5	SCCPs/ MCCPs	N.D.	N.D.	N.D.	46200

PIP (3:1) is a mixture of isomers with different numbers of isopropyl groups attached at different locations. The structural formula of PIP (3:1) is shown in Fig. 4. Py-Screener Ver. 3 can detect PIP (3:1) isomers with 1 to 4 attached isopropyl groups (iPr:x, where x is 1 to 4), but it determines PIP (3:1) concentrations in terms of the most common isomer, iPr:3. iPr:3 is normally detected as 7 to 8 isomer peaks (Fig. 5), and sample levels are determined as the total of these peak areas.

Approximately 1300 mg/kg of PIP (3:1) was detected in the capacitor plastic. US TSCA regulations specify a limit of 1000 mg/kg (as of January 2026) for PIP (3:1) in products, so the analysis shows the condenser plastic may violate the regulations. For reference, another example analysis of PIP (3:1) in plastic is described in Application News No. 01-00191.



R=CH(CH₃)₂
x≧1 y≧1 z≧1

Fig. 4 Structural Formula of PIP (3:1)

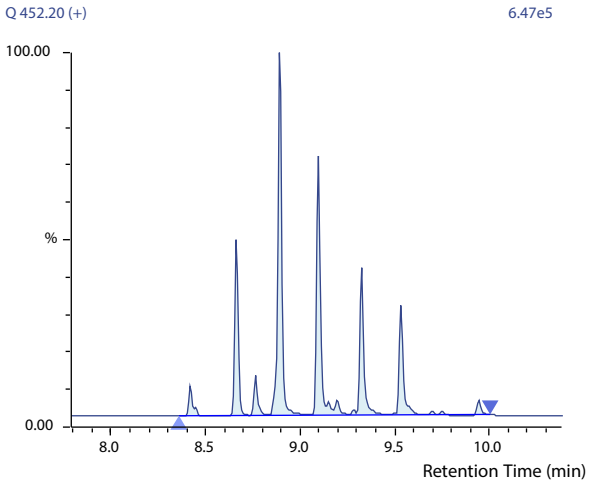


Fig. 5 SIM Chromatogram of PIP (3:1) (Capacitor Plastic)

UV-328 was detected in the PVC sample. The SIM chromatogram of UV-328 is shown in Fig. 6. The concentration of UV-328 was approximately 70 mg/kg. EU regulations on POPs specify a limit of 100 mg/kg (as of January 2026) for UV-328 in products, so the PVC sample may violate the regulations. For reference, another example analysis of UV-328 in plastic is described in Application News No. 01-00488. Approximately 700 mg/kg of PIP (3:1) was also detected in the PVC sample. US TSCA regulations specify a limit of 1000 mg/kg (as of January 2026) for PIP (3:1) in products, so the analysis shows the PVC sample may violate the regulations.

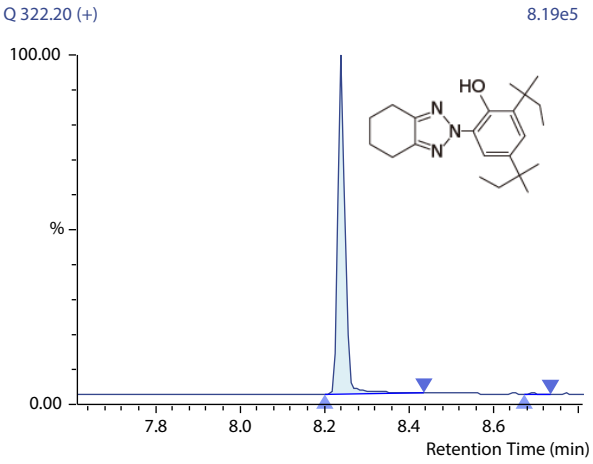


Fig. 6 SIM Chromatogram of UV-328 (PVC Sample)

Two DP structural isomers, syn-DP and anti-DP, were detected in the ABS sample (Fig. 7). The concentration of DP in the ABS sample, which was determined by summing the area of both peaks, was under 500 mg/kg. EU regulations on POPs specify a limit of 1000 mg/kg (as of January 2026) for DP in products, so the analysis shows the amount of DP in the ABS sample was within the permissible range. Another example analysis of DP in plastic is presented in Application News No. 01-00488.

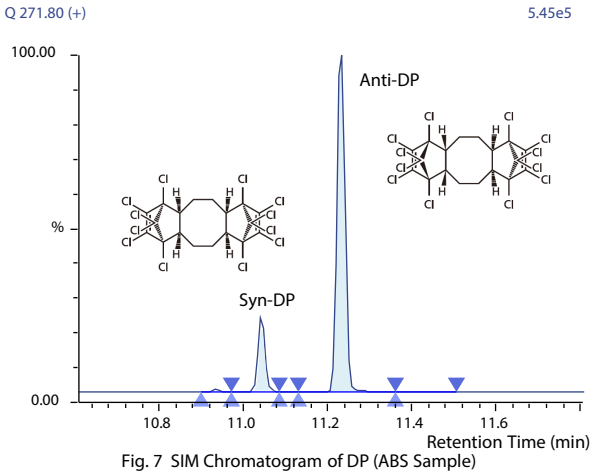


Fig. 7 SIM Chromatogram of DP (ABS Sample)

SCCPs and MCCPs are mixtures of isomers and congeners of chlorinated linear hydrocarbons of different carbon chain lengths. They are characterized by their unique chromatogram profile. Fig. 8 shows an example of an SCCP, and Fig. 9 shows an example of an MCCP. Py-Screener Ver.3 uses EI (not NCI) to detect and quantitate SCCPs and MCCPs. It does not differentiate between individual compounds and quantifies them as a sum (SCCPs/MCCPs)*1.

A chromatogram profile that is unique to SCCPs and MCCPs was detected in the analysis of the insulator cord (Fig. 10). The concentration of SCCPs and MCCPs exceeded 40,000 mg/kg, which strongly suggests the intentional use of SCCPs or MCCPs in the sample. Both SCCPs and MCCPs have been designated for elimination from products under Annex A of the POPs Convention.

*1 Long-chain chlorinated paraffins (LCCPs) may be detected as SCCPs/MCCPs if present.

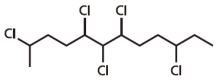


Fig. 8 Example SCCP
Molecular Formula: $C_{12}H_{21}Cl_5$

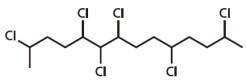


Fig. 9 Example MCCP
Molecular Formula: $C_{14}H_{24}Cl_6$

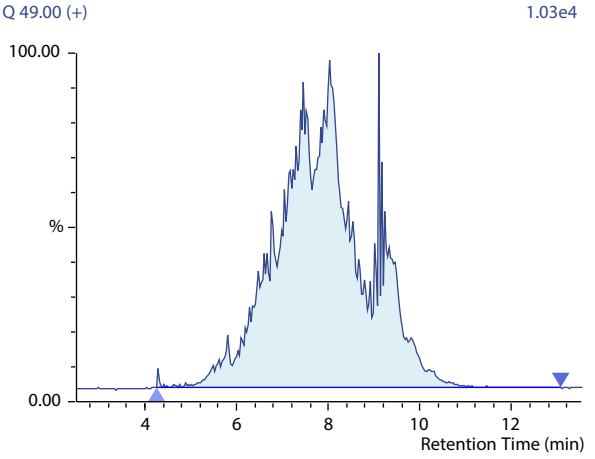


Fig. 10 SIM Chromatogram of SCCPs and MCCPs (Insulator Cord)

■ Conclusion

Py-Screener Ver. 3 successfully determined in samples the concentrations of the regulated substances PIP (3:1), UV-328, DP, and SCCPs and MCCPs. Normally, SCCP and MCCP levels are tested using NCI, but Py-Screener Ver. 3 uses EI. This enables it to test for not only SCCPs and MCCPs but also phthalate esters, brominated flame retardants, and other regulated substances in just one analysis. In addition, by using the relative correction factors linked to DEHP in the phthalate ester reference material, the levels of these regulated substances were determined without the need for the corresponding reference materials.

Py-Screener Ver. 3 can also create a screening program that addresses substance restrictions under the RoHS Directive, the US TSCA, and the POPs Convention.

<References>

1) IEC 62321-8:2017, *Determination of certain substances in electrotechnical products –Part 8: Phthalates in polymers by gas chromatography-mass spectrometry(GC-MS), gas chromatography mass spectrometry using a pyrolyzer/thermal desorption accessory (Py/TD-GC-MS)*
2) IEC 62321-3-3:2021, *Determination of certain substances in electrotechnical products - Part 3-3: Screening - Polybrominated biphenyls, polybrominated diphenyl ethers and phthalates in polymers by gas chromatography-mass spectrometry using a pyrolyser/thermal desorption accessory (Py/TD-GC-MS)*
3) Persistent, Bioaccumulative, and Toxic (PBT) Chemicals under TSCA
4) European Commission. *Commission Delegated Regulation (EU) 2025/843 of 5 May 2025 amending Annex I to Regulation (EU) 2019/1021 of the European Parliament and of the Council as regards UV-328(C/2025/2567)*
5) European Commission. *Commission Delegated Regulation (EU) …/... amending Regulation (EU) 2019/1021 of the European Parliament and of the Council as regards dechlorane plus (C/2025/2887).*
6) European Commission. *Commission Regulation (EU) 2015/2030 of 13 November 2015 amending Regulation (EC) No 850/2004 of the European Parliament and of the Council on persistent organic pollutants as regards Annex I (Text with EEA relevance)(32015R2030)*
7) European Commission. *Commission Delegated Regulation (EU) …/... amending Regulation (EU) 2019/1021 of the European Parliament and of the Council as regards medium chain chlorinated paraffins(Ares/2025/10131503)*

<Related Application News Articles>

1. Analysis of PIP (3:1) in Plastic by Py/TD-GC-MS, Application News No. 01-00191
2. Analyzing UV-328 and Dechlorane Plus in Plastic by Pyrolyzer/ Thermal Desorption-GC-MS, Application News No. 01-00488

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