## Optimization of extraction methods for non-targeted analysis of food contact materials

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Background 재활용 페트병의 배신…"새 병보다 발암물질 더 나왔다" 종이 빨대도 친환경 아냐...90%서 영원한 화학물질 'PFAS' 검출

- Recently growing environmental and health concerns surrounding the use of eco-friendly food contact materials (FCMs).
- Inadequate safety assessment of unknown hazardous substances that may unintentionally or intentionally migrate from FCMs to food.

Methods

### 1. Sample information

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No.	Material type	Sample number	No.	Material type	Sample number
1	PE	12	8	Silicone	1
2	HDPE	1	9	Pulp	1
3	LDPE	1	10	PE/PA	1
4	PP	6	11	PE/PP	1
5	OP	1	12	OP/PA/PET	1
6	PVDC	1	13	Paper/PE	1
7	Aluminum	1			

### 2. Extraction procedure



Washing

# Cleaning Extraction



## 3. LC-MS/MS conditions

	LC	Condition					
Inst	trument	1290 Infinity II UPLC system (Agilent)					
Column		ACQUITY UPLC BEH C18 (1.7 µm, 2.1×100mm)					
Mobile phase		<ul><li>(A) 0.1 % acetic acid in water</li><li>(B) 0.1 % acetic acid in methanol</li></ul>					
Flow rate		0.3 mL/min					
Injection volume		2 µL					
Credient	Time (min)	0	2	15	18	18.1	23
Gradient	Solvent B (%)	2	2	98	98	2	2

MS/MS	Condition
Instrument	6546 Q-TOF (Agilent)
lon polarity	Positive/Negative
Gas temp.	300 °C
MS range	150 - 1,000 m/z
Acquisition mode	Data dependent (Top 4 precursors)
Collision energy	0.03 × m/z + 15

#### 4. Data processing





Figure 1. Proposed workflow for extracting non-intentionally intended substances in FCMs.

#### 2. Optimization of extraction conditions



Figure 2. The number of detected features across the tested conditions: (a) extraction solvents of water, methanol, and ethanol, and (b) extraction times of 30, 45, and 60 min for PS1, PS2, PE1, and PE2 samples.

### 3. Non-targeted analysis results



Figure 3. Workflow of the non-targeted analysis for FCMs and detected or identified features according to each workflow step. The color of the text on the right-hand side of the figure corresponds to the color of the arrow in the workflow.

Table 1.	. Identified	compounds	by the	non-targeted	analysis
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No.	Compound name	RT (min)	Exact mass (m/z)	lon form
1	Tripropylene glycol monobutyl ether	12.67	271.1880	[M+Na]+
2	Dihexyl adipate	15.73	337.2374	[M+Na]+
3	Sucrose	1.60	365.1056	[M+Na]+

Acknowledgements: This research was supported by a grant (24192MFDS044) from Ministry of Food and Drug Safety in 2024.

