XXVI ENCONTRO

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GC-MS SCREENING METHOD FOR THE IDENTIFICATION OF SEMI-VOLATILE COMPOUNDS IN BIO-BASED AND BIODEGRADABLE FOOD PACKAGING MATERIALS

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INTRODUCTION

Bio-based and biodegradable plastics are being used for food packaging applications as an alternative to conventional plastics derived from petroleum feedstocks due to the environmental pollution originated by the use of traditional petroleum-based non- biodegradable polymers [1, 2].

Bio-based polymers like other food contact materials may transfer low molecular weight constituents into the food and therefore represent a risk for the consumers' health. However, the chemical safety of these sustainable materials has been scarcely studied [1].

In the present work, a gas chromatography coupled to gass spectrometry (GC-MS) screening method for the identification of semi-volatile components in bio-based and biodegradable food packaging materials was developed. Six different plastic materials labeled as biodegradable, bio-based or compostable were collected to carried out the study.

EXPERIMENTAL

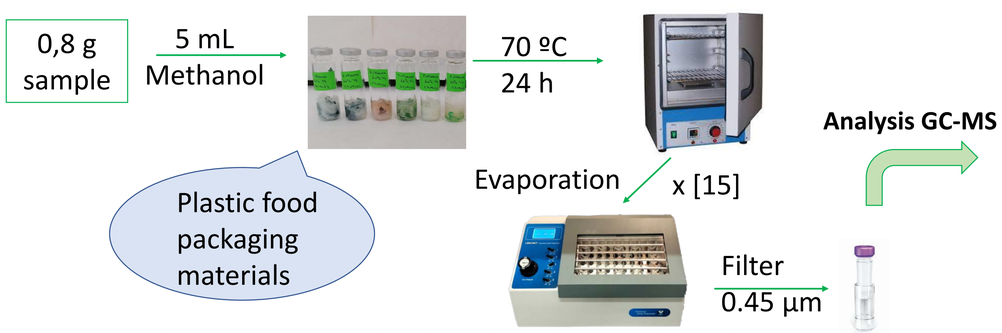

Figure 1. Sample extraction procedure (sample code: 1, 4, 5, 7, 8, F).

Figure 2. GC-MS.

Column	*Rxi-5SilMS (30 m x 0.25 mm, 0.25 µm)*
Injection Volume	1 *µL*
Carrier gas flow (He)	1 mL/ min
Full scan range	35-500 m/z
Injector Temperature	300 °C
Transfer line Temperature	300 °C
Ramp Temperature	40-300 °C
Mode of injection	Splitless

Table 1. Chromatographic and spectrometric conditions.

RESULTS AND DISCUSSION

Tr/ min	Compound	CAS	m/z	SI	RSI	1	4	5	7	8	F
8.52	Cyclohexane,isocyanate*	3173-53-3	67, 82, 97	706	836		x				
10.64	2-Methoxyacetate	3938-96-3	45, 88				x				
10.8	Isobutylhydrazine	42504-87-0	45, 88	681	706			x			x
10.95	1,4-Dioxane-2,5-dione,3,6-dimethyl	95-96-5	56	768	781			x			
12.43	Ethanol,2-phenoxy*	122-99-6	94, 138	829	921		x				
13.32	Nonanoic acid	112-05-0	45, 60, 73					x			
14.29	6,10-dimethylundecan-2-one	1604-34-8	43, 57	616	678					x	
15.28	5-Decyne-4,7,diol,2,4,7,9-tetramethyl	126-86-3	43, 109, 151					x			
16.05	2,6-di-tert-butyl-p-benzoquinone*	719-22-2	135, 177, 220	896	907					x	
17.3	1, 6-Dioxacyclododecane-7,12-dione	777-95-7	55, 84, 100, 129				x	x			
17.5	Dodecanoic acid	143-07-7	60, 73	927	954			x			
17.76	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	43, 71				x			x	
17.78	Diethyl phthalate*	84-66-2	149	930	933			x			
18	Decyl methoxyacetate	259141-02-1	45	833	863			x			
18.45	Benzophenone*	119-61-9	77, 105	945	954			x			
18.46	Tributyl phosphate*	126-73-8	99, 155	802	879					x	
18.68	Octyl ether	629-82-3	57, 71,	846	886	x				x	
19.23	Methanone, (1-hydroxycyclohexyl)phenyl	947-19-3	81, 99					x			
19.35	1,15-Pentanediol	14722-40-8	82	741	880					x	
19.43	Methyl tetradecanoate	124-10-7	74, 87	846						x	
21.32	1-Hexadecanol	3665382-4	55, 69, 83, 97	926	946	x					
21.65	7,9-di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	175, 205	863	888					x	
21.8	Hexadecanoix acid, methyl ester*	112-39-0	74, 87, 143	907	910	x				x	
22.4	n-Hexadecanoic acid	57-10-3	73, 129	924	927	x		x		x	x
22.86	Isopropyl palmitate	142-91-6	43, 102, 239, 256	914	921	x					
22.87	Octadecanal	638-66-4	43, 57, 82, 96	891	927					x	
23.55	1-Octadecanol	112-92-5	55, 69, 83, 97	916	953	x					
22.56	2,4(3H,5H)-Furandione,3,5-dimethyl	5460-81-1	56, 100, 128	675	728						x
23.95	Methyl stearate	112-61-8	74, 87	872	905	x				x	
24.02	N-Methylthioacetamide	5310-10-1	56, 89	581	821						x
24.03	2-[2´-(n-phthalimido)ethoxy]phenylacetic acid	115149-67-2	130, 174	768	973	x					
24.15	9,12-Octadecanoic acid (Z,Z)	60-33-3	67, 81, 95	918	924		x				
24.23	trans-13-Octadecanoic acid	693-71-0	55, 69					x			
24.42	Octadecanoic acid	57-11-4	43, 55, 73	803	825		x	x		x	
24.57	Hexadecanamide*	629-54-9	59, 72	912	915	x		x			
25.09	Hexadecanoic acid,2-hydroxyethyl ether	4219-49-2	98, 104, 239	833	853	x					
25.15	Tributyl acetylcitrate*	77-90-7	129, 185, 259	879	932	x				x	
25.73	2,4-Pentanediol, 3-methyl	5683-44-3	45, 56, 100								x
25.9	12-Hydroxystearic acid	106-14-9	55, 87, 197	738	771				x		
26.37	9-Octadecenamide	301-02-0	59, 72	914	916	x	x				
26.57	Octadecanamide	124-26-5	59, 72	865	874	x		x			
27.66	Palmitin,2-mono	23470-00-0	98, 239	881	885		x				
27.8	Bis(2-ethylhexyl) phthalate	117-81-7	149, 167	921	931	x					
28.17	9-Octadecenamide	301-02-0	59, 72				x				
29.99	13-Docosenamide*	112-84-5	59,72	887	907	x	x			x	
30.14	Squalene*	111-02-4	69, 81	918	920	x					
33.1	Tetradecanoic acid, hexadecyl ester	2599-01-01	57, 229	845	850			x			
36.03	Irgafos 168*	31570-04-4	57, 147, 441			x					
39.3	Tris(2,4-di-tert-butylphenyl)phosphate	95906-11-9	57, 191, 316	532	548	x					
39.34	methyl 3,5-dicyclohexyl-4-hydroxybenzoate	55125-23-0	191, 316	539	585					x	
39.87	Irganox 1076*	2082-79-3	57, 147, 219	700	718	x					

Table 2. Compounds identified by GC-MS. (* substances confirmed with analytical standard)

- Biobased, biodegradable and compostable materials were extracted for the screening analysis by GC-MS.
- **IAS**: **I**ntentionally **A**dded **S**ubstances to the polymer such as antioxidants (Irgafos 168, Irganox 1076), slip agents (hexadecanamide, erucamide), lubricants (octadecanoic acid), or plasticizers (tributyl acetylcitrate, diethyl phthalate) were identified and some of them confirmed with analytical standard.
- **NIAS: N**on **I**ntentionally **A**dded **S**ubstances such as 2,6-di-tert-butyl-p-benzoquinone, 1, 6-dioxacyclododecane-7,12-dione or 7,9-di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione were identified.

CONCLUSIONS

The proposed method allowed the rapid identification of potential semi-volatile migrants in the bio-based packaging materials. It could be used as a screening tool for the selection of relevant substances the migration of which should further be studied in specific migration tests.

REFERENCES

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