Simultaneous analysis of trace polymer additives in plastic beverage packaging by solvent sublation followed by high-performance liquid chromatography

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Table S1 Polymer additives

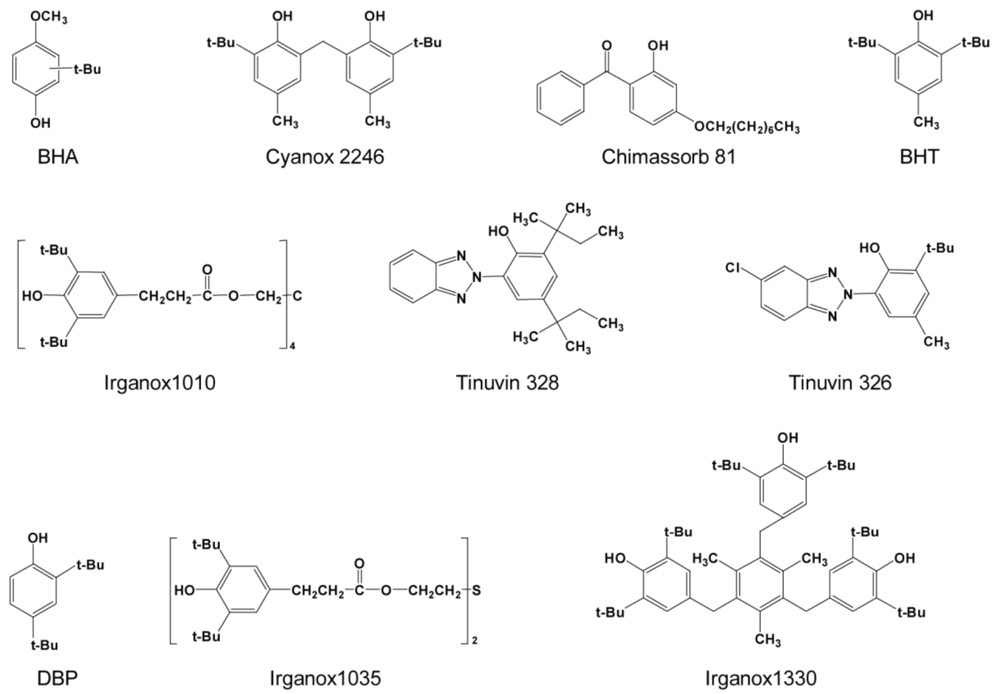
Chemicals	Polymer additives	CAS No.	Source	Purity	SML[a](mg/kg)[13,26]
BHA	antioxidant	25013-16-5	Sigma	> 99%	30
Cyanox 2246	antioxidant	119-47-1	TCI	> 99%	1.5
Chimassorb 81	antioxidant	1843-05-6	Sigma	> 98%	
BHT	antioxidant	128-37-0	Alfa Aesar	> 99%	3
Irganox 1010	antioxidant	6683-19-8	Sigma	> 98%	
DBP	antioxidant	96-76-4	Sigma	> 99%	
Irganox1035	antioxidant	41484-35-9	TCI	> 98%	2.4
Irganox 1330	antioxidant	1709-70-2	Sigma	> 99%	
Tinuvin 328	UV absorber	25793-55-1	Sigma	> 98%	
Tinuvin 326	UV absorber	3896-11-5	Sigma	> 98%	

[a]SML, specific migration levels.

Table S2 Commercial beverage packages and corresponding simulants

No.	Beverage package	Beverage Type	Beverage simulant	Type of polymer material
1#	Red tea	Normal (pH > 4.5)	Distilled water	PET
2#	Mineral water-1	Normal (pH > 4.5)	Distilled water	PET
3#	Mineral water-2	Normal (pH > 4.5)	Distilled water	PET
4#	Mineral water-3	Normal (pH > 4.5)	Distilled water	PET
5#	Mineral water-4	Normal (pH > 4.5)	Distilled water	PET
6#	Milk-1	Normal (pH > 4.5)	Distilled water	LDPE
7#	Milk-2	Normal (pH > 4.5)	Distilled water	PP
8#	Milk-3	Normal (pH > 4.5)	Distilled water	LDPE
9#	Pear juice	Normal (pH > 4.5)	Distilled water	PET
10#	Lemon juice	Normal (pH > 4.5)	Distilled water	PET
11#	Chocolate drink	Normal (pH > 4.5)	Distilled water	LDPE
12#	Yogurt-1	Acidic (pH ≤ 4.5)	Acetic acid solution (3%)	PP
13#	Yogurt-2	Acidic (pH ≤ 4.5)	Acetic acid solution (3%)	LDPE
14#	Yogurt-3	Acidic (pH ≤ 4.5)	Acetic acid solution (3%)	LDPE
15#	Fruit yogurt	Acidic (pH ≤ 4.5)	Acetic acid solution (3%)	PE
16#	Carbonated drink	Acidic (pH ≤ 4.5)	Acetic acid solution (3%)	PET
17#	Vinegar drink	Acidic (pH ≤ 4.5)	Acetic acid solution (3%)	LDPE

PET, polyethylene terephthalate; LDPE, low density polyethylene; PP, polypropylene; PE, polyethylene.



*BHA: butylated hydroxyanisole (M_w=180.25)

Cyanox 2246: 2,2'-methylenebis(4-methyl-6-terl-bulyphenol) (M_w=340.50)

Chimassorb 81: 2-Hydroxy-4-(octyloxy)benzophenone (M_w=326.00)

BHT: 2,6-di-tert-butyl-4-methylphenol (M_w=220.36)

Irganox 1010: pentaerythritol tetrakis 3,5-di-*tert*-butyl-4-hydroxydro-cinnamate (M_w=1177.67)

Tinuvin 328: 2-(2*H*-Benzotriazol-2-yl)-4,6-di-tert-pentylphenol (M_w=316.81)

Tinuvin 326: 2-*tert*-Butyl-6-(5-chloro-2H-benzotiazol-2-yl)-4-methyl-phenol (M_w=351.50)

DBP: 2,4-di-tert-butylphenol (M_w=206.32)

Irganox1035: 2,2'-Thiodiethyl Bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate (M_w=642.93)

Irganox 1330: 1,3,5-Trimethyl-2,4,6- tris(3,5-di-tert-butyl-4-hydroxy-benzyl) benzene (M_w=775.22)

Fig. S1. Chemical structures of ten polymer additives.

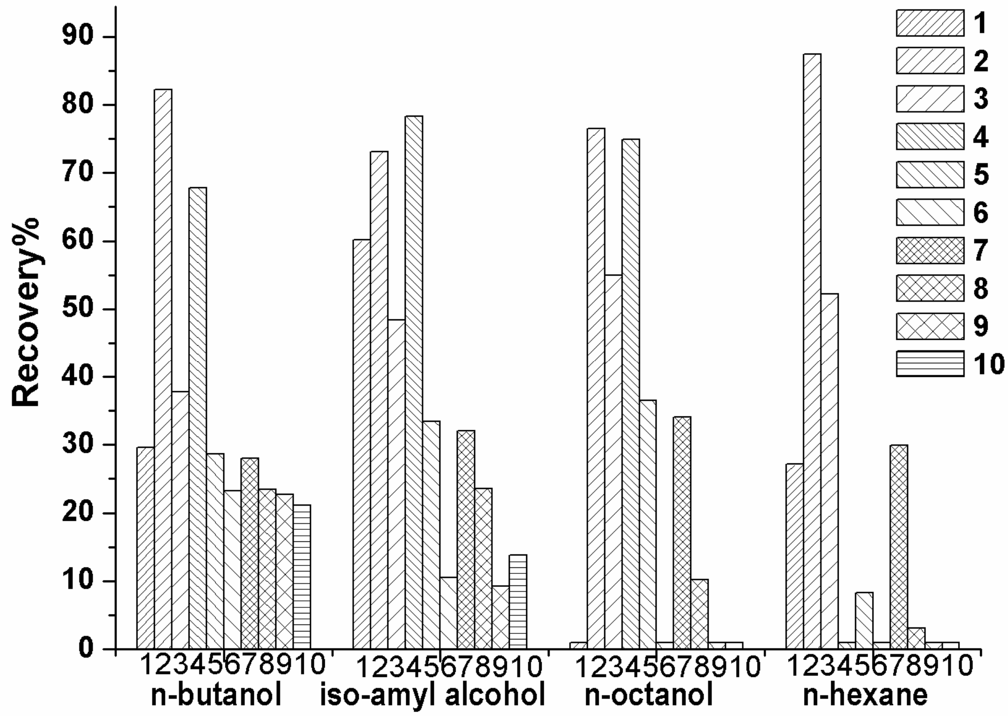


Fig. S2 The comparison of separation efficiency for different sublation solvents.

pH = 7, m_{NaCl} = 0 g, flow rate = 40 ml/min, flotation time = 30 min. (1. BHA; 2. DBP; 3. BHT; 4. Cyanox 2246; 5. Chimassorb 81; 6. Irganox 1035; 7. Tinuvin 326; 8. Tinuvin 328; 9. Irganox 1010; 10. Irganox 1330)

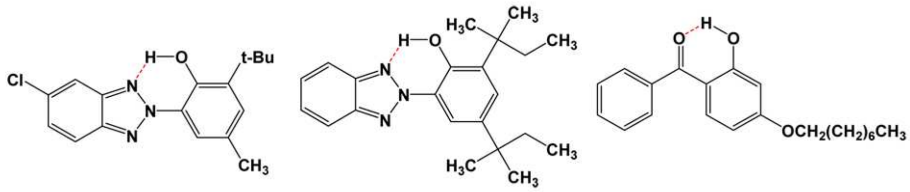


Fig. S3 Intra-molecular hydrogen bonds in Tinuvin 326, Tinuvin 328 and Chimassorb 81.

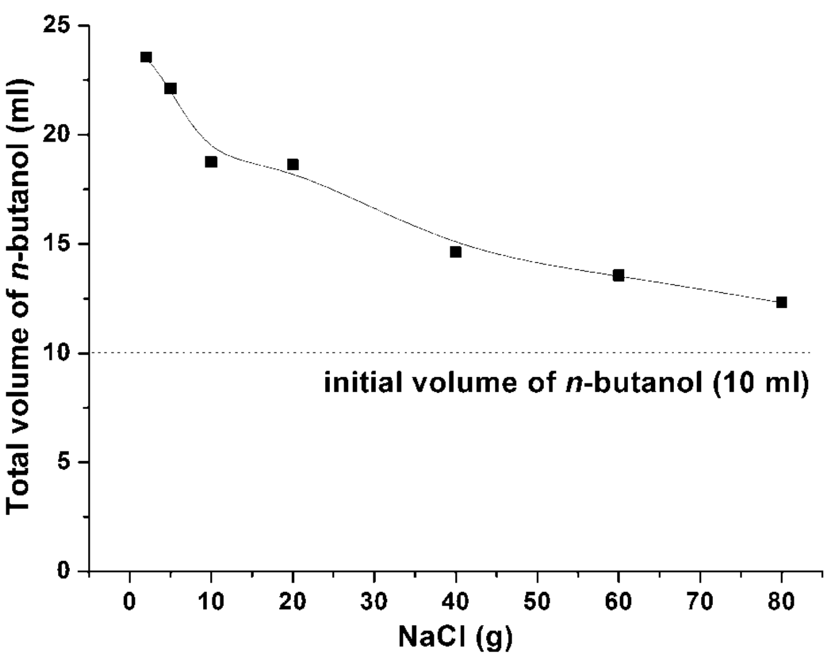


Fig. S4 Effect of NaCl addition on the consumption volume of *n*-butanol.

Sublation solvent is *n*-butanol, pH = 3, flow rate = 40 ml/min, flotation time = 30 min.

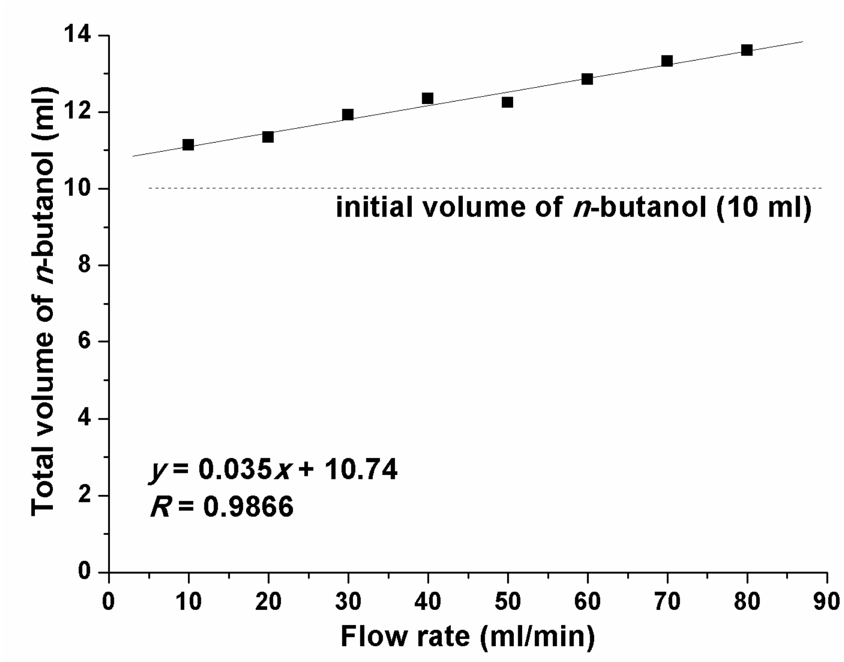


Fig. S5 Effect of nitrogen flow rate on the consumption volume of *n*-butanol. Sublation solvent is *n*-butanol, pH = 3, m_{NaCl} = 80 g, flotation time = 30 min.

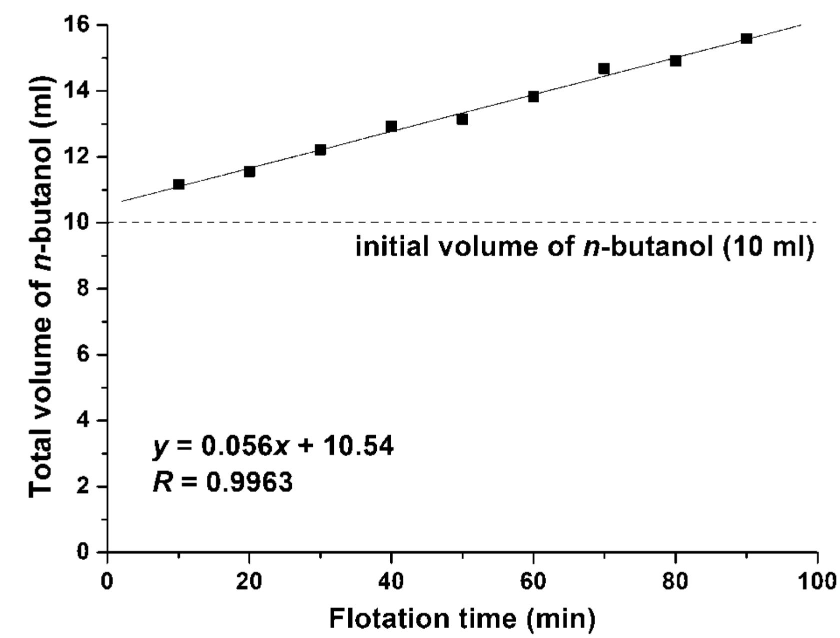


Fig. S6 Effect of sublation time on the consumption volume of *n*-butanol. Sublation solvent is *n*-butanol, pH = 3, m_{NaCl} = 80 g, flow rate = 60 ml/min.

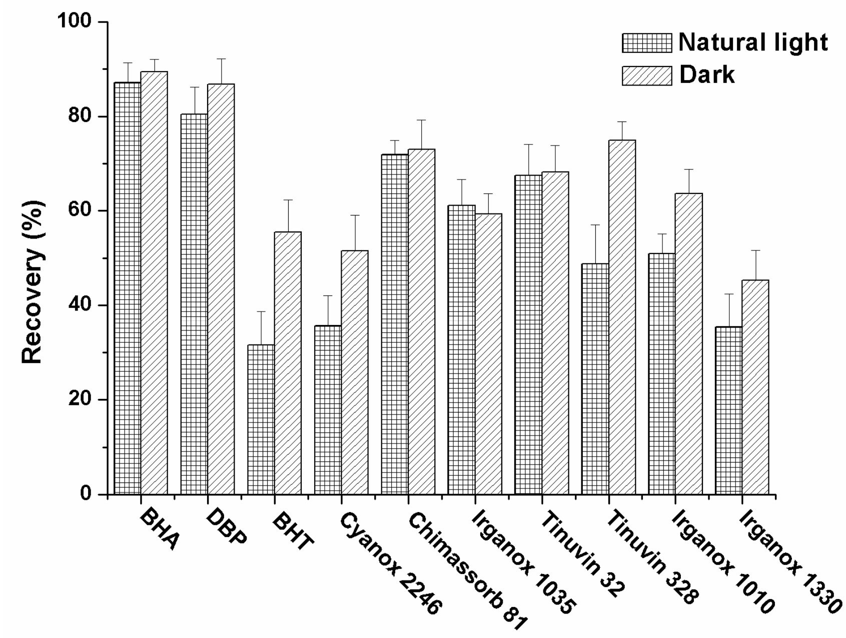


Fig. S7 Effect of light condition on solvent sublation (*n* = 3).

Sublation solvent is *n*-butanol, pH = 3, m_{NaCl} = 80 g, flow rate = 60 ml/min, flotation time = 60 min.