

Supplementary Material

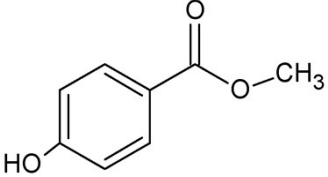
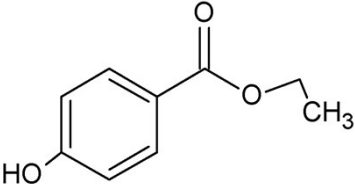
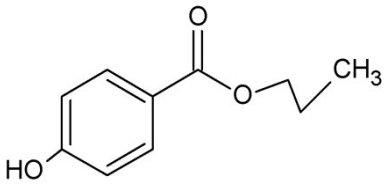
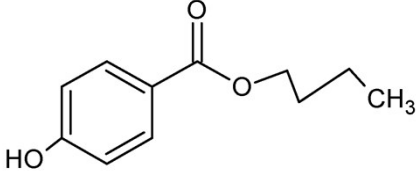
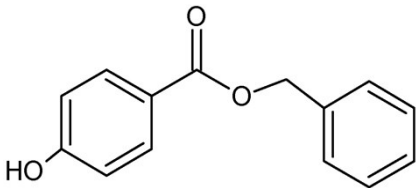
Optimization of double-vortex-assisted matrix solid-phase dispersion for the rapid determination of paraben preservative residues in leafy vegetables

Chun-Ju Yang^a, Wu-Hsun Chung^{a,b}, Wang-Hsien Ding^{a,*}

**^a Department of Chemistry, National Central University,
Chung-Li 320, Taiwan**

**^b Department of Chemical Engineering, Army Academy ROC,
Chung-Li 320, Taiwan**

Table S1. Name (abbreviation), chemical structure, physical and chemical properties of five parabens used for the method development and validation.

Name (Abbreviation):	Structure	MW (g/mol)	Molecular formula	pK _a	LogK _{ow}	Vapor pressure mm Hg (25°C)
Methyl-paraben (MeP)		152.1476	C ₈ H ₈ O ₃	8.5	1.96	2.37×10 ⁻⁴
Ethyl-paraben (EtP)		166.1742	C ₉ H ₁₀ O ₃	8.5	2.47	9.29×10 ⁻⁵
Propyl-paraben (PrP)		180.2008	C ₁₀ H ₁₂ O ₃	7.91	3.04	3.07×10 ⁻⁴
Butyl-paraben (BuP)		194.2275	C ₁₁ H ₁₄ O ₃	8.47	3.57	2.51×10 ⁻⁴
Benzyl-paraben (BzP)		228.2438	C ₁₄ H ₁₂ O ₃	8.5	3.70	No data available

The values of pK_a, Log Kow and vapor pressure are reported in PubChem <https://pubchem.ncbi.nlm.nih.gov/compound/>

Table S2. Analysis of variance (ANOVA) for Factorial Multilevel Categorical design

Source	Sum of Squares ($\times 10^{11}$)	df	Mean Square ($\times 10^{11}$)	F Value	<i>p</i> -value Prob > F
Model	117.92	5	39.31	39.73	< 0.0001*
A-Sorbent	6.19	2	6.19	3.79	0.1367
B-Extracting solvent	91.07	1	91.07	92.03	< 0.0001*
C- Extraction mechanic force	6.53	1	6.53	6.59	0.0332*
BC	20.34	1	20.34	20.55	0.0019*

df: Degree of freedom.

*Significant

Table S3. Experimental results based on the Box-Behnken design for DVA-MSPD and their total peak area

Run	Vortex time (min)	C18 amount (g)	MeOH (mL)	Total Peak Area ($\times 10^5$)
1	15	0.6	5	33.52
2	10	1	5	29.96
3	10	1	10	40.97
4	5	1	7.5	42.37
5	5	0.6	5	33.24
6	15	1	7.5	34.73
7	5	0.6	10	37.87
8	10	0.6	7.5	41.45
9	10	0.6	7.5	41.10
10	10	0.6	7.5	41.51
11	15	0.2	7.5	55.13
12	10	0.2	5	46.81
13	10	0.2	10	48.36
14	15	0.6	10	36.84
15	5	0.2	7.5	48.49

Table S4. Analysis of variance (ANOVA) of the Box-Behnken design for total peak area

Source	Sum of Squares ($\times 10^9$)	df	Mean Square ($\times 10^9$)	F Value	<i>p</i> -value Prob > F
Model	6463.5	9	718.2	105.0	< 0.0001*
A-Vortex time	3.9	1	3.9	0.6	0.4860
B-C18	3219.3	1	3219.3	470.7	< 0.0001*
C-MeOH	525.5	1	525.5	76.8	0.0003*
AB	509.6	1	509.6	74.5	0.0003*
AC	4.3	1	4.3	0.6	0.4632
BC	223.9	1	223.9	32.7	0.0023*
A ²	49.9	1	49.9	7.3	0.0425
B ²	920.8	1	920.8	134.7	< 0.0001*
C ²	857.2	1	857.2	126.4	< 0.0001*
Lack-of-Fit	33.2	3	11.1	2.36	0.431

df: Degree of freedom.

*Significant

Table S5. Spiked recoveries (%) of individual target analyte for each experimental condition.

Run	Vortex time (min)	C18 amount (g)	MeOH (mL)	MeP	EtP	(%) PrP	BuP	BzP
1	15	0.6	5	35.7	34.5	53.8	68.1	76.3
2	10	1	5	37.4	37.1	49.8	59.1	68.8
3	10	1	10	33.9	42.0	72.8	80.0	80.5
4	5	1	7.5	38.1	51.6	77.1	77.9	81.0
5	5	0.6	5	31.8	33.6	57.5	69.9	71.6
6	15	1	7.5	38.0	35.5	60.8	68.0	75.2
7	5	0.6	10	38.4	45.5	64.1	72.6	80.2
8	10	0.6	7.5	48.3	43.5	74.9	76.4	82.4
9	10	0.6	7.5	48.4	56.7	76.9	72.8	77.7
10	10	0.6	7.5	53.4	55.7	78.0	71.4	75.2
11	15	0.2	7.5	77.8	80.4	82.9	94.8	97.9
12	10	0.2	5	67.3	75.3	74.8	80.1	85.5
13	10	0.2	10	82.6	70.3	80.4	81.1	83.7
14	15	0.6	10	69.0	59.9	64.4	65.2	66.1
15	5	0.2	7.5	86.1	74.7	77.0	81.8	84.1