Supplementary Material

Characterization of Plant Volatiles Reveals Distinct Metabolic Profiles and Pathways among 12 Brassicaceae Vegetables

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Table S1. VOCs identified by GC-Q-TOF/MS.

Compound	RT, min	RI[a]	Mono MW	Formula	CAS	Group	VIP[b]	*p*-Value[c]
3-Decyne	10.47	1001	138.1408	$C_{10}H_{18}$	2384-85-2	Alkane	1.4	5.86×10^{-6}
Nonadecane	22.17	1407	268.313	$C_{19}H_{40}$	629-92-5	Alkane	1.1	8.31×10^{-6}
Phenylethyl Alcohol	14.03	1116	122.0731	$C_8H_{10}O$	60-12-8	Alcohol	1.1	7.83×10^{-6}
1-Penten-3-ol	2.67	<800	86.0732	$C_5H_{10}O$	616-25-1	Alcohol	1.1	2.29×10^{-5}
3-(Z)-Hexenol	6.22	856	100.0188	$C_6H_{12}O$	928-96-1	Alcohol	1.1	2.83×10^{-5}
2-(E)-Hexenol	6.52	867	100.0188	$C_6H_{12}O$	928-95-0	Alcohol	1.0	5.60×10^{-6}
1-Hexanol	6.6	870	100.0188	$C_6H_{12}O$	111-27-3	Alcohol	1.1	6.12×10^{-6}
2-(E)-Hexenal	6.13	852	98.0731	$C_6H_{10}O$	6728-26-3	Aldehyde	1.2	7.86×10^{-6}
3-Hexenal	4.72	<800	98.0731	$C_6H_{10}O$	4440-65-7	Aldehyde	1.2	8.69×10^{-6}
2,4-(E,E)-Hexadienal	7.82	914	96.0575	C_6H_8O	142-83-6	Aldehyde	1.3	3.84×10^{-6}
(E)-4-Oxohex-2-enal	9.39	965	112.0524	$C_6H_8O_2$	2492-43-5	Aldehyde	1.3	7.79×10^{-6}
2-Hexenol acetate	11.05	1019	142.0994	$C_8H_{14}O_2$	10094-40-3	Ester	1.24	1.75×10^{-5}
(3Z)-3-Hexenyl acetate	10.75	1010	142.0993	$C_8H_{14}O_2$	1708-82-3	Ester	1.6	1.35×10^{-4}
Hexyl acetate	10.98	1017	144.1150	$C_8H_{16}O_2$	142-92-7	Ester	1.3	8.38×10^{-6}
(4E)-4-Hexenyl propionate	13.6	1102	156.1150	$C_9H_{16}O_2$	-	Ester	1.2	3.57×10^{-6}
(4E)-4-Hexenyl butyrate	14.93	1147	170.1307	$C_{10}H_{18}O_2$	69727-41-9	Ester	1.3	1.45×10^{-5}
(4E)-4-Hexenyl hexanoate	20.58	1347	198.1620	$C_{12}H_{22}O_2$	88552-98-1	Ester	1.3	6.28×10^{-6}
Pentyl acetate	7.9	917	130.0993	$C_7H_{14}O_2$	628-63-7	Ester	1.3	2.14×10^{-5}
Eucalyptol	11.54	1035	154.1358	$C_{10}H_{18}O$	470-82-6	Monoterpene	1.2	7.08×10^{-6}
3-Carene	8.47	936	136.1252	$C_{10}H_{16}$	13466-78-9	Monoterpene	1.0	1.38×10^{-5}
p-Cymene	11.32	1028	134.1095	$C_{10}H_{14}$	99-87-6	Monoterpene	1.4	1.26×10^{-5}
Camphene	8.97	1052	136.1252	$C_{10}H_{16}$	79-92-5	Monoterpene	1.2	6.12×10^{-6}
β-Pinene	10.24	993	136.1252	$C_{10}H_{16}$	127-91-3	Monoterpene	1.3	7.83×10^{-6}
D-Limonene	11.46	1033	136.1252	$C_{10}H_{16}$	5989-27-5	Monoterpene	1.6	5.94×10^{-6}
γ-Terpinene	12.36	1061	136.1252	$C_{10}H_{16}$	99-85-4	Monoterpene	1.2	1.12×10^{-5}
Allyl Isothiocyanate	6.9	882	99.0142	C_4H_5NS	57-06-7	Isothiocyanate	1.7	3.82×10^{-6}

3-Butenyl isothiocyanate	9.905	982	113.0299	C_5H_7NS	3386-97-8	Isothiocyanate	1.7	4.38×10^{-6}
3-Methylbutyl isothiocyanate	12.29	960	129.0612	$C_6H_{11}NS$	628-03-5	Isothiocyanate	1.4	4.69×10^{-6}
4-Methylpentyl isothiocyanate	15.41	1163	143.0769	$C_7H_{13}NS$	17608-07-0	Isothiocyanate	1.1	5.98×10^{-6}
Pentyl isothiocyanate	13.47	1098	129.0612	$C_6H_{11}NS$	629-12-9	Isothiocyanate	1.3	6.20×10^{-6}
Hexyl isothiocyanate	16.51	1200	143.0769	$C_7H_{13}NS$	4404-45-9	Isothiocyanate	1.1	3.16×10^{-6}
Heptyl isothiocyanate	18.33	1264	157.0925	$C_8H_{15}NS$	4426-83-9	Isothiocyanate	1.2	4.22×10^{-6}
3-Methylthiopropyl isothiocyanate	19.64	1311	147.0176	$C_5H_9NS_2$	505-79-3	Isothiocyanate	1.5	7.83×10^{-6}
4-Methylthio-3-butenyl isothiocyanate	22.46	1419	159.0176	$C_6H_9NS_2$	51598-96-0	Isothiocyanate	1.2	6.34×10^{-6}
Phenethyl isothiocyanate	23.7	1467	163.0456	C_9H_9NS	2257-09-2	Isothiocyanate	1.3	5.53×10^{-6}
Dimethyl disulfide	3.58	<800	93.9911	$C_2H_6S_2$	624-92-0	Sulphur compounds	1.1	5.39×10^{-6}
Dimethyl trisulfide	9.51	969	125.9631	$C_2H_6S_3$	3658-80-8	Sulphur compounds	1.0	7.60×10^{-6}
1-(Methylsulfanyl)-1,3-butadiene	5.86	842	100.0347	C_5H_8S	10574-97-7	Sulphur compounds	1.0	2.26×10^{-6}
3-Methylisothiazole	10.64	1006	99.0143	C_4H_5NS	693-92-5	Sulphur compounds	1.5	9.45×10^{-6}
4,5-Dimethylthiazole	14.245	1124	113.0299	C_5H_7NS	3581-91-7	Sulphur compounds	1.6	4.12×10^{-6}
4-Propylthiazole	13.01	1083	127.0456	C_6H_9NS	41981-60-6	Sulphur compounds	1.6	3.30×10^{-5}
3-Butenenitrile	2.38	<800	67.0422	C_4H_5N	109-75-1	Nitrile	1.5	5.21×10^{-6}
3-Pentenenitrile	3.955	<800	81.0578	C_5H_7N	4635-87-4	Nitrile	1.4	1.01×10^{-5}
2-Methylbutanenitrile	5.81	840	83.0735	C_5H_9N	18936-17-9	Nitrile	1.2	1.51×10^{-4}

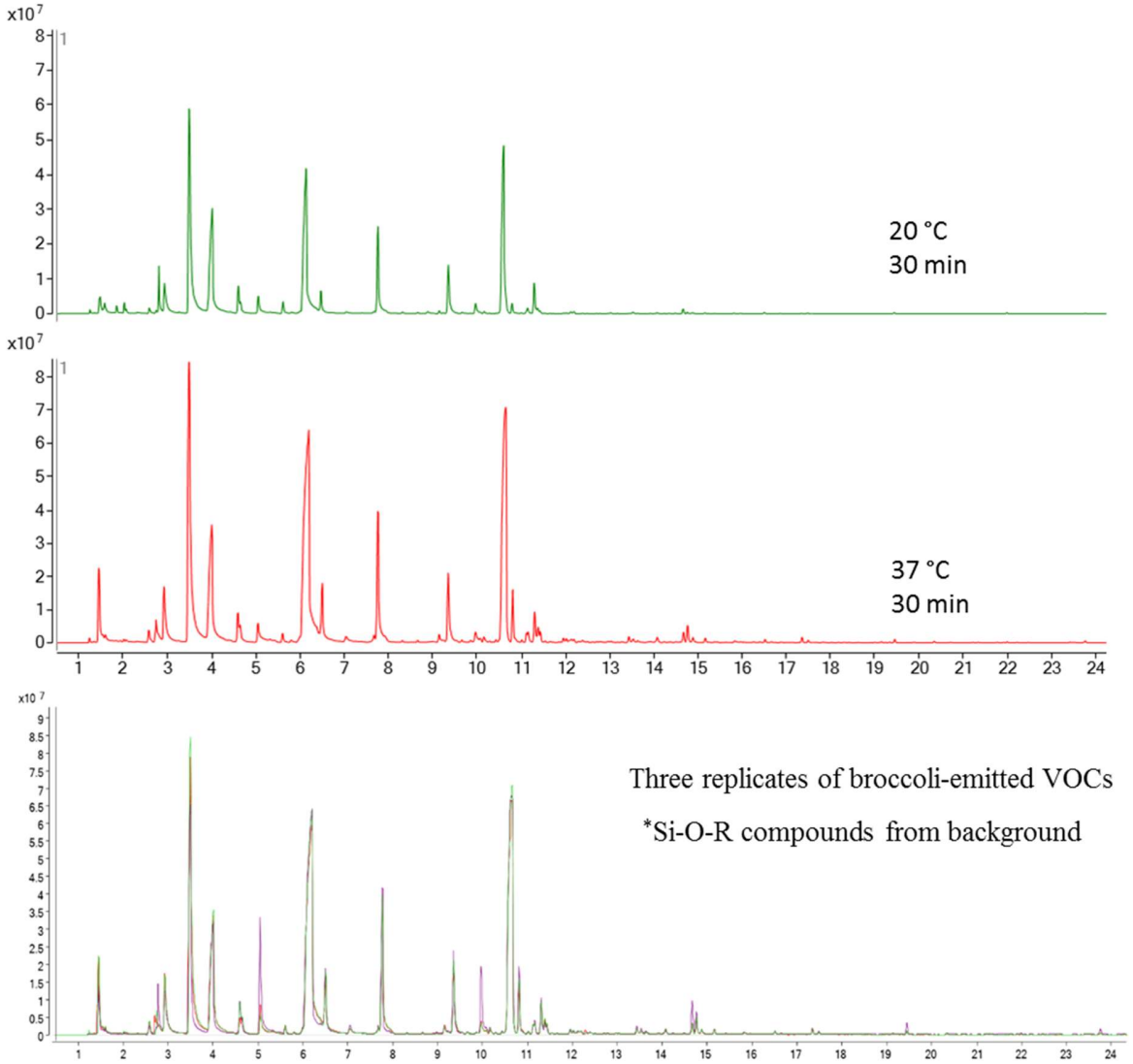

Figure S1a. Comparison of extraction temperature.

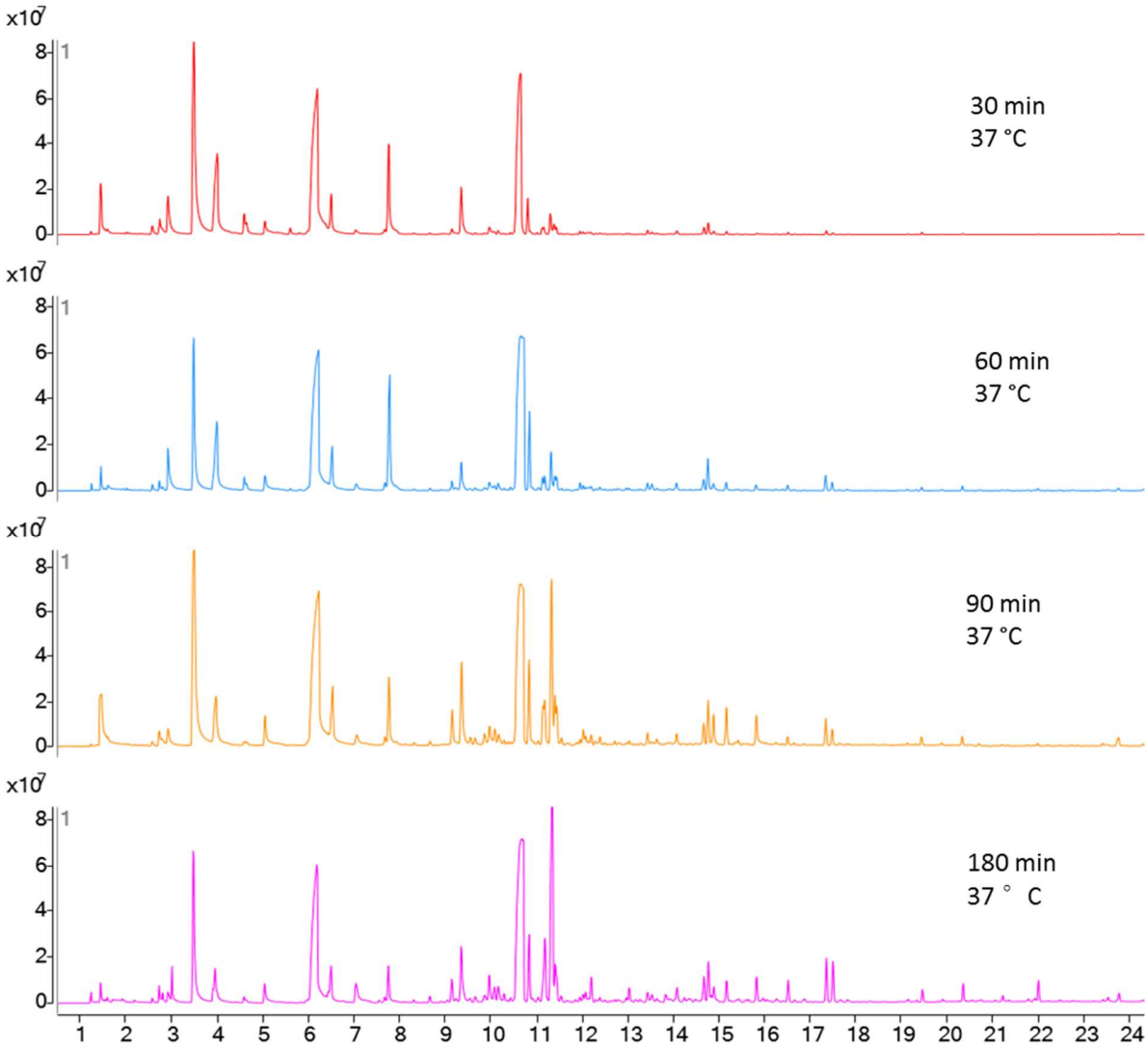

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Figure S1b. Comparison of extraction time.

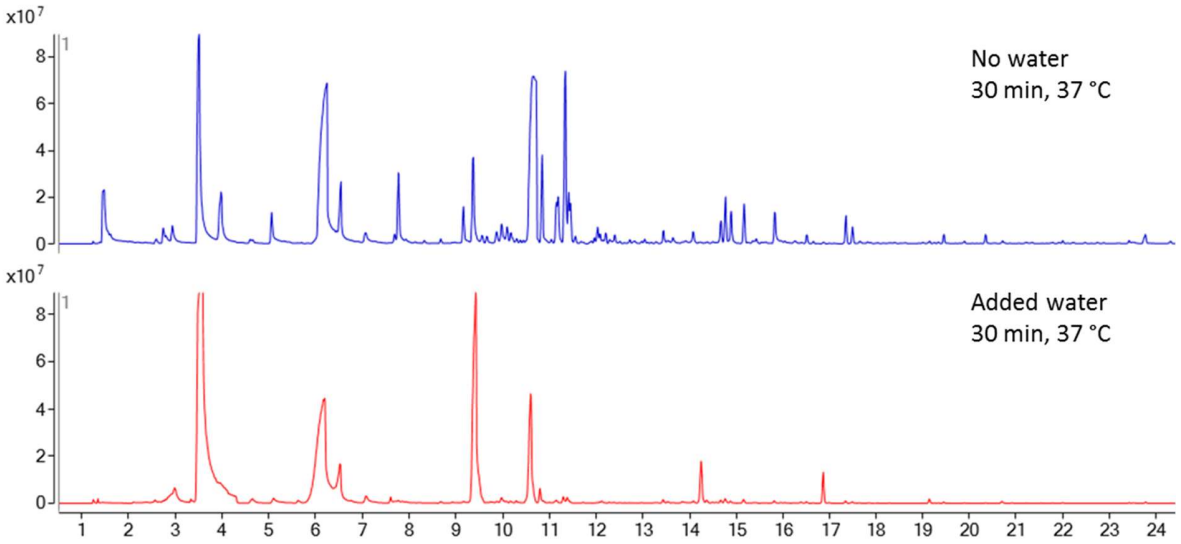

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Figure S1c. Evaluation of addition of water.

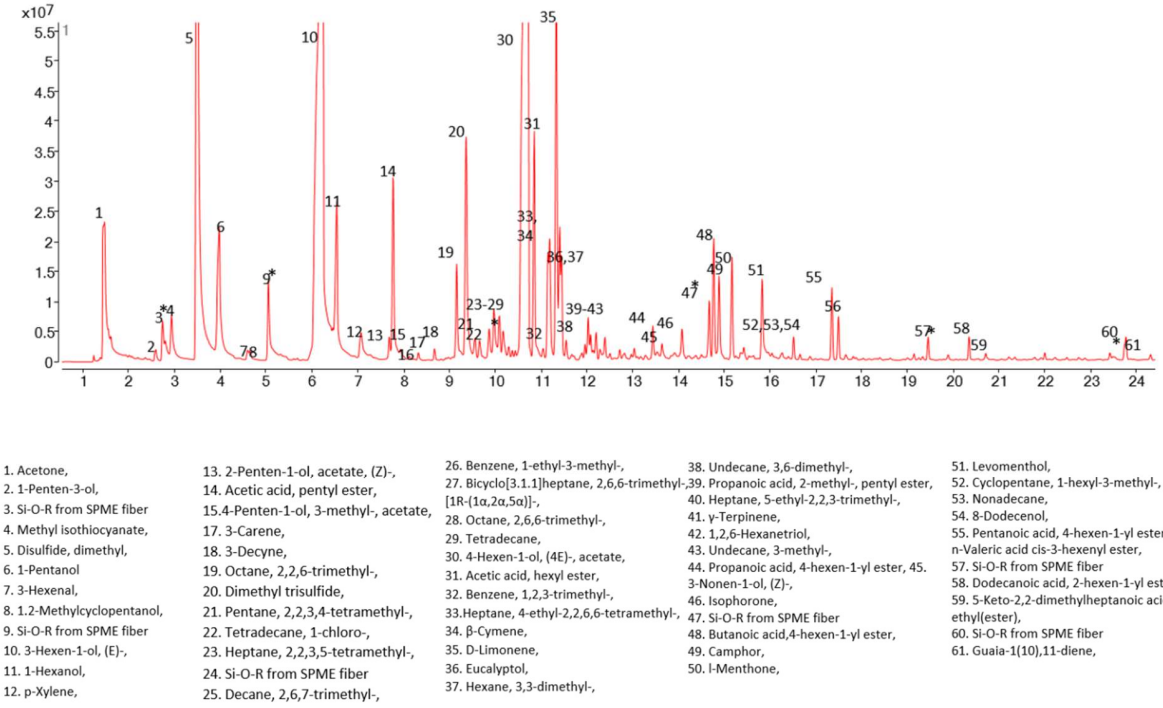

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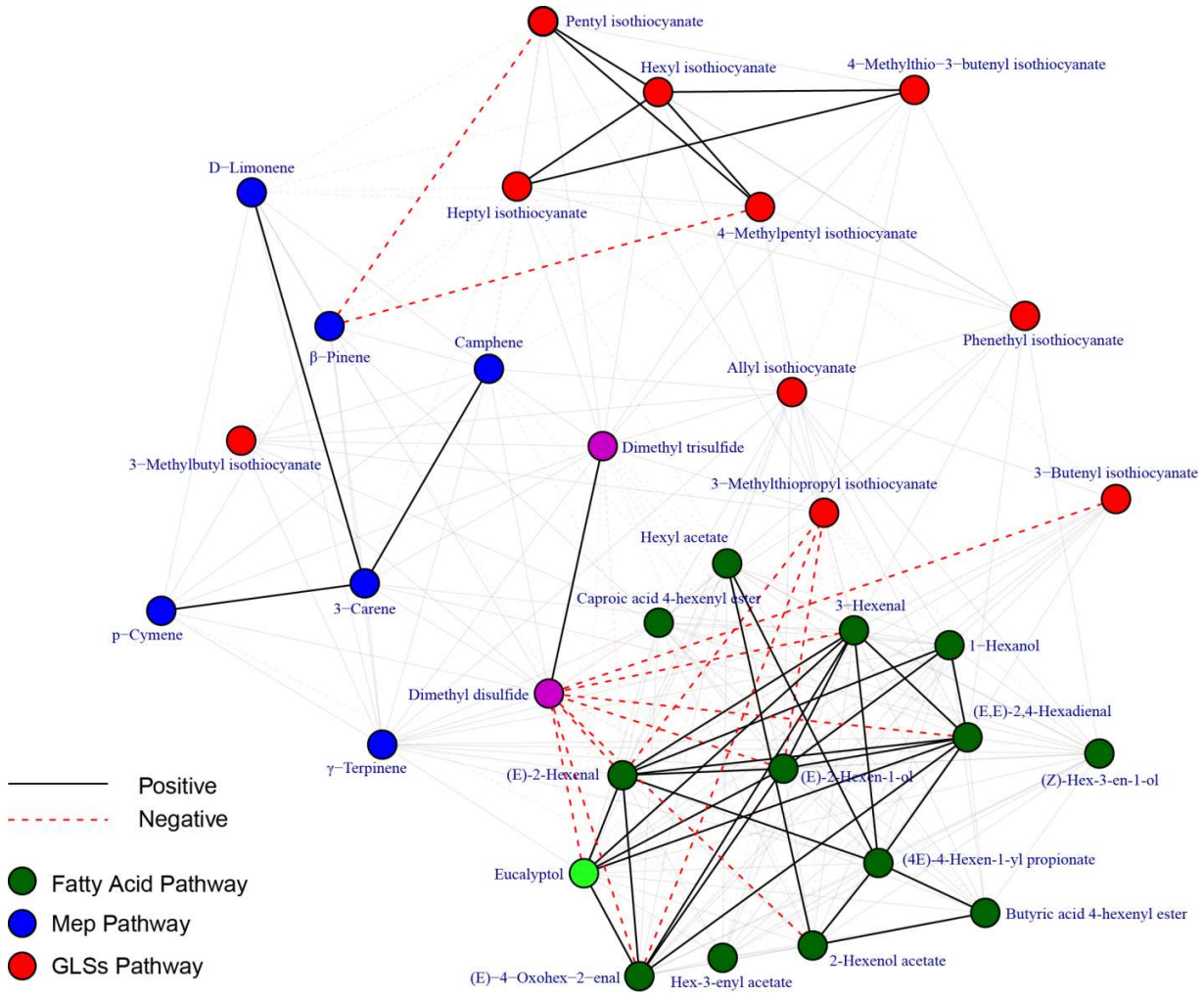
Figure S1d. The chromatogram under the optimized conditions.

Figure S1. Representative chromatograms of VOCs emitted from broccoli: (**a**) comparison of extraction temperature, (**b**) comparison of extraction time, (**c**) evaluation of addition of water, and (**d**) the chromatogram under the optimized conditions.



Note: Significant correlations ($p < 0.05$) were plotted between VOCs. The positive correlation with a correlation coefficient higher than 0.8 is shown by the black solid line. The negative correlation with a correlation coefficient lower than –0.5 is shown by the red dashed line.

Figure S2. Network plot of Spearman correlations of VOCs in 12 Brassicaceae vegetables.

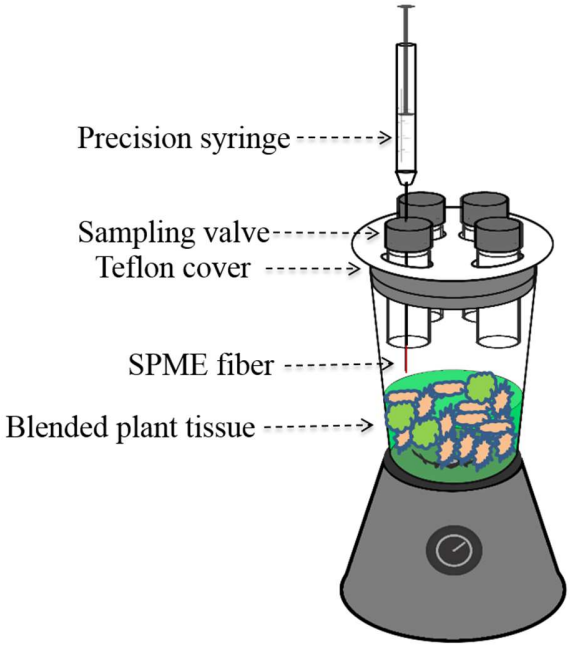


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Figure S3. Diagram of the sampling device.

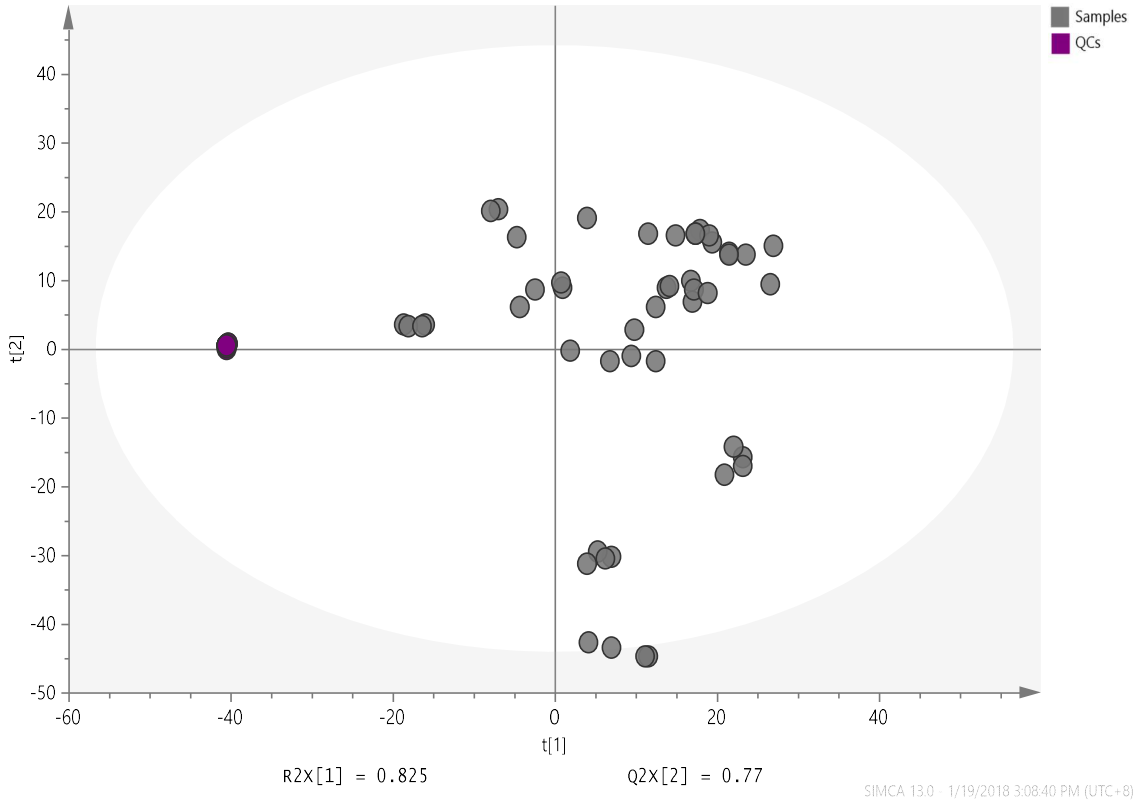

Figure S4. Evaluation of QCs' reproducibility through PCA analysis.