

Table S1 The information of chemicals used in this study.

Chemicals	Manufacturer information
Ethyl decanoate	TCI Chemical Industry Development Co., Ltd
High purity water	Hangzhou Wahaha Group Co., Ltd.
<i>n</i> -Alkane mixtures (C7-C40)	Shanghai Yuanye Biotechnology Co., Ltd.

Table S2 The identified volatile compounds in sweet and floral aroma black tea during the entire manufacturing process by using GC-IMS.

No.	Compounds	Formula s	MW	RI	Rt [sec]	Dt [a.u.]	Types	Peak intensities						Comment	
								Fresh leaves	Withering	Shaking	Rolling	Fermentatio n	First drying		Final firing
#3	Linalool	C ₁₀ H ₁₈ O	154.3	1102.1	497.755	1.21735	Alcohols	4197.53 ±	6624.05 ±	7584.27 ±	6017.60 ±	5979.39 ±	3424.66 ±	4269.92 ±	
								318.58d	211.01b	152.96a	90.58c	68.58c	59.03e	96.77d	
#32	2-Butoxyethanol	C ₆ H ₁₄ O ₂	118.2	898.8	262.525	1.19921	Alcohols	82.27 ±	104.16 ±	128.79 ±	62.82 ±	97.06 ± 8.70b	37.96 ±	41.10 ±	
								11.63c	8.56b	9.22a	5.44d		2.20e	2.28e	
#36	(E)-2-Hexen-1-ol	C ₆ H ₁₂ O	100.2	848.3	233.41	1.51715	Alcohols	2460.34 ±	2208.67 ±	2533.77 ±	2586.43 ±	2979.77 ±	1929.30 ±	1782.84 ±	
								50.04c	44.94d	44.44bc	63.06b	57.78a	48.16e	50.61f	
#46	(E)-3-Hexen-1-ol	C ₆ H ₁₂ O	100.2	866.9	243.374	1.23957	Alcohols	542.42 ±	567.47 ±	612.00 ±	766.70 ±	804.38 ±	1135.88 ±	1092.52 ±	
								33.75d	34.66d	18.12c	6.53b	15.55b	23.00a	32.23a	
#68	Pentan-1-ol-M	C ₅ H ₁₂ O	88.1	762.7	190.332	1.25248	Alcohols	390.45 ±	368.40 ±	295.79 ±	139.40 ±	159.42 ± 4.50e	217.80 ±	224.22 ±	Monomer
								5.60a	7.50b	6.74c	0.10f		5.47d	7.92d	
#78	Pentan-1-ol-D	C ₅ H ₁₂ O	88.1	762.9	190.397	1.50823	Alcohols	620.69 ±	808.90 ±	651.11 ±	285.62 ±	266.76 ±	112.65 ±	161.01 ±	Dimer
								17.54c	18.55a	30.01b	4.80d	9.91d	3.86f	11.22e	
#79	3-Methylbutan-1-ol-D	C ₅ H ₁₂ O	88.1	727.3	175.966	1.48408	Alcohols	146.14 ±	203.68 ±	198.25 ±	124.35 ±	103.49 ±	26.15 ±	22.37 ±	Dimer
								2.20b	3.72a	6.58a	2.23c	3.93d	1.28e	0.27e	
#82	2-Methyl-1-propanol	C ₄ H ₁₀ O	74.1	624	142.881	1.36641	Alcohols	417.28 ±	707.02 ±	584.19 ±	193.18 ±	165.94 ± 3.31e	59.88 ±	39.28 ±	
								9.68c	22.53a	8.70b	0.85d		7.50f	2.11g	
#91	3-Methylbutan-1-ol-M	C ₅ H ₁₂ O	88.1	729.8	176.98	1.24282	Alcohols	38.10 ±	37.30 ±	37.84 ±	42.45 ±	54.20 ± 1.95a	33.31 ±	32.05 ±	Monomer
								5.38bc	2.05bc	1.67bc	1.61b		0.78cd	2.27d	

#92	2-Methylbutan-1-ol-M	C ₅ H ₁₂ O	88.1	732.4	178.047	1.22947	Alcohols	9.43 ± 3.01bc	14.41 ± 0.39a	13.72 ± 0.60a	10.66 ± 0.67b	9.79 ± 0.23b	8.85 ± 0.90bc	7.15 ± 1.01c	Monomer
#93	Pentan-2-ol	C ₅ H ₁₂ O	88.1	711.6	169.626	1.45245	Alcohols	50.08 ± 4.16c	39.33 ± 2.68c	83.04 ± 0.50b	318.04 ± 12.48a	303.48 ± 15.30a	42.70 ± 2.87c	24.57 ± 4.34d	
#96	tert-Butanol	C ₄ H ₁₀ O	74.1	508.9	111.816	1.14369	Alcohols	205.17 ± 14.14d	287.84 ± 4.32c	290.77 ± 7.36c	346.03 ± 20.33b	502.28 ± 3.61a	363.08 ± 19.92b	134.52 ± 6.70e	
#97	n-Hexanol	C ₆ H ₁₄ O	102.2	873.8	247.073	1.32819	Alcohols	306.55 ± 9.83b	394.72 ± 5.82a	233.06 ± 6.00d	234.77 ± 3.66d	251.96 ± 3.78c	242.72 ± 10.14cd	205.00 ± 6.66e	
#98	2-Methylbutan-1-ol-D	C ₅ H ₁₂ O	88.1	724.2	174.74	1.46541	Alcohols	110.32 ± 0.75b	139.30 ± 11.07a	139.68 ± 4.67a	115.55 ± 5.65b	85.93 ± 2.30c	21.28 ± 1.06d	22.55 ± 3.38d	Dimer
#12	(E, E)-2,4-Heptadienal	C ₇ H ₁₀ O	110.2	1011. 1	366.97	1.19696	Aldehydes	242.65 ± 10.58e	369.57 ± 8.33c	503.59 ± 26.27b	463.64 ± 42.30b	696.06 ± 45.22a	497.47 ± 12.90b	291.73 ± 4.72d	
#20	Benzaldehyde-M	C ₇ H ₆ O	106.1	957.1	312.341	1.14868	Aldehydes	1624.48 ± 22.83b	1660.72 ± 7.69a	1445.84 ± 8.64c	713.06 ± 13.04ef	735.44 ± 22.34e	697.23 ± 2.37f	1208.33 ± 4.81d	Monomer
#21	Benzaldehyde-D	C ₇ H ₆ O	106.1	957.1	312.341	1.46512	Aldehydes	4647.47 ± 55.90a	4610.32 ± 16.57a	2960.66 ± 59.22b	343.06 ± 15.73d	339.22 ± 10.67d	231.70 ± 5.90e	831.77 ± 7.93c	Dimer
#25	Heptanal-M	C ₇ H ₁₄ O	114.2	899.4	263.11	1.3379	Aldehydes	334.58 ± 8.14g	429.66 ± 9.06c	353.94 ± 0.53f	390.10 ± 7.69e	407.33 ± 6.54d	636.53 ± 12.39a	524.25 ± 8.14b	Monomer
#26	Heptanal-D	C ₇ H ₁₄ O	114.2	898.8	262.531	1.69914	Aldehydes	333.20 ± 7.62e	678.68 ± 21.98b	528.88 ± 19.97d	539.89 ± 22.51d	571.95 ± 20.66cd	970.29 ± 43.51a	612.64 ± 24.27c	Dimer
#33	(E)-Hept-2-enal	C ₇ H ₁₂ O	112.2	951.1	307.204	1.25402	Aldehydes	59.98 ± 3.40c	56.69 ± 0.57c	73.66 ± 1.66b	62.28 ± 4.04c	93.81 ± 5.49a	68.17 ± 3.56b	28.89 ± 2.59d	Unidentified
#42	Octanal	C ₈ H ₁₆ O	128.2	1004. 1	356.92	1.4119	Aldehydes	77.12 ± 6.58c	100.09 ± 5.82ab	107.24 ± 5.83a	42.31 ± 0.44d	44.50 ± 3.92d	103.55 ± 7.81ab	96.77 ± 4.05b	
#45	Nonanal	C ₉ H ₁₈ O	142.2	1107. 6	505.747	1.4811	Aldehydes	260.91 ± 16.71c	217.58 ± 14.43d	240.52 ± 5.27cd	169.26 ± 13.46e	187.61 ± 9.40e	398.32 ± 21.96a	370.41 ± 17.11b	

#49	Hexanal-M	C ₆ H ₁₂ O	100.2	790	202.166	1.26454	Aldehydes	375.24 ±	364.57 ±	357.82 ± 3.54f	404.74 ±	379.42 ±	654.44 ±	505.86 ±	Monomer
								4.56de	7.35ef		8.94c	3.64d	5.20a	8.75b	
#50	Hexanal-D	C ₆ H ₁₂ O	100.2	791.6	203.03	1.56406	Aldehydes	558.22 ±	524.33 ±	691.35 ±	1560.52 ±	1602.18 ±	1649.07 ±	1034.17 ±	Dimer
								40.85e	7.97e	11.25d	25.34b	14.51ab	48.68a	13.45c	
#52	(E)-2-Pentenal-M	C ₅ H ₈ O	84.1	750	185.17	1.10704	Aldehydes	167.83 ±	126.74 ±	200.59 ±	373.04 ±	385.83 ± 0.95c	572.04 ±	493.03 ±	Monomer
								4.40f	2.40g	6.52e	4.63d		9.32a	13.92b	
#53	(E)-2-Pentenal-D	C ₅ H ₈ O	84.1	748.8	184.703	1.36125	Aldehydes	659.10 ±	597.51 ±	1193.92 ±	1394.62 ±	1624.23 ±	787.80 ±	689.54 ±	Dimer
								41.11e	22.76f	2.38c	40.34b	33.64a	2.13d	9.71e	
#57	Pentanal-M	C ₅ H ₁₀ O	86.1	695	162.869	1.18413	Aldehydes	119.99 ±	107.49 ±	70.67 ± 2.68e	84.38 ±	81.81 ± 2.78d	194.45 ±	120.06 ±	Monomer
								1.34b	4.36c		3.08d		0.81a	2.82b	
#58	Pentanal-D	C ₅ H ₁₀ O	86.1	693	162.078	1.4225	Aldehydes	304.78 ±	331.11 ±	285.87 ±	240.04 ±	279.09 ±	353.63 ±	144.13 ±	Dimer
								12.88c	3.06b	3.11d	4.02e	11.97d	15.88a	7.03f	
#59	2-Methylbutanal	C ₅ H ₁₀ O	86.1	660.9	152.809	1.39939	Aldehydes	1905.56 ±	2362.14 ±	2271.56 ±	2454.12 ±	2369.34 ±	2975.94 ±	3139.16 ±	
								17.68f	18.97d	19.60e	16.13c	8.06d	46.82b	43.45a	
#60	3-Methylbutanal	C ₅ H ₁₀ O	86.1	640.5	147.308	1.41143	Aldehydes	1289.39 ±	1516.07 ±	1502.55 ±	1697.11 ±	1581.10 ±	1814.31 ±	1944.14 ±	
								42.46f	5.94e	14.43e	9.25c	15.29d	33.62b	9.08a	
#64	Butanal	C ₄ H ₈ O	72.1	548.7	122.555	1.28401	Aldehydes	1124.16 ±	1538.96 ±	1745.00 ±	1532.83 ±	1304.15 ±	1294.82 ±	1405.48 ±	
								35.30e	38.81b	26.93a	20.39b	6.62d	43.71d	120.81c	
#76	2-Methyl-2-pentenal-D	C ₆ H ₁₀ O	98.1	823	219.874	1.49791	Aldehydes	405.34 ±	608.65 ±	534.71 ±	65.08 ±	98.58 ± 4.79d	34.42 ±	53.69 ±	Dimer
								27.22c	21.67a	16.00b	2.81e		3.37f	2.80ef	
#81	2-Methyl-2-pentenal-M	C ₆ H ₁₀ O	98.1	822.2	219.396	1.16162	Aldehydes	118.81 ±	138.54 ±	125.03 ±	50.20 ±	59.32 ± 1.21d	33.27 ±	34.00 ±	Monomer
								5.42c	2.37a	4.64b	3.39e		1.78f	1.61f	
#1	(Z)-3-Hexenyl butyrate	C ₁₀ H ₁₈ O ₂	170.3	1240.	696.712	1.43164	Esters	100.06 ±	122.72 ±	251.05 ±	364.28 ±	364.96 ±	170.21 ±	208.81 ±	
				4				5.19e	5.08e	20.48b	10.29a	28.79a	2.46d	15.50c	
#2	Methyl Salicylate	C ₈ H ₈ O ₃	152.1	1230.	681.86	1.20064	Esters	349.49 ±	990.68 ±	1501.37 ±	1559.08 ±	1886.24 ±	925.23 ±	1673.94 ±	
				1				51.70e	54.19d	58.96c	94.92bc	53.57a	121.12d	20.71b	

#14	Butanoic acid, 2-ethyl-3-methyl, ethyl ester-M	C ₉ H ₁₈ O ₂	158.2	981	332.671	1.38724	Esters	1377.86 ±	1361.29 ±	1405.68 ±	1818.18 ±	1255.55 ±	2324.57 ±	2150.03 ±	Monomer
								34.04de	7.62e	13.21d	20.25c	45.35f	8.38a	11.66b	
#15	Butanoic acid, 2-ethyl-3-methyl, ethyl ester-D	C ₉ H ₁₈ O ₂	158.2	982.3	333.802	1.82352	Esters	2385.39 ±	3684.75 ±	3345.28 ±	1902.76 ±	608.70 ±	2227.20 ±	3164.57 ±	Dimer
								55.11d	33.84a	38.72b	99.91f	41.12g	91.34e	107.40c	
#22	Ethyl 3-hydroxybutanoate	C ₆ H ₁₂ O ₃	132.2	938.1	296.123	1.17298	Esters	317.60 ±	336.74 ±	315.70 ±	590.82 ±	767.55 ± 8.07a	140.09 ±	83.41 ±	
								6.59d	2.84c	10.19d	10.50b		9.67e	5.97f	
#23	Hexyl formate-M	C ₇ H ₁₄ O ₂	130.2	921.5	281.934	1.28921	Esters	73.47 ± 2.00f	78.00 ±	229.27 ±	994.01 ±	1025.64 ±	555.54 ±	520.70 ±	Monomer
									1.90f	6.93e	10.54b	22.00a	9.02c	6.95d	
#24	Hexyl formate-D	C ₇ H ₁₄ O ₂	130.2	920.1	280.775	1.6803	Esters	53.15 ± 5.17f	56.22 ±	202.21 ±	2435.46 ±	2132.44 ±	263.14 ±	292.17 ±	Dimer
									2.42f	2.96e	31.66a	26.51b	4.02d	6.71c	
#44	Ethyl hexanoate	C ₈ H ₁₆ O ₂	144.2	1001.7	353.466	1.3425	Esters	35.90 ± 3.07c	22.92 ±	26.57 ±	80.44 ±	58.40 ± 3.47b	27.76 ±	29.39 ±	
									2.22e	1.05de	4.39a		2.19de	1.35d	
#55	n-Propyl acetate-D	C ₅ H ₁₀ O ₂	102.1	707	167.771	1.47689	Esters	130.17 ±	84.81 ±	144.72 ±	1042.50 ±	1047.13 ±	327.49 ±	159.36 ±	Dimer
								5.23d	1.04e	7.00cd	23.96a	11.37a	24.95b	15.73c	
#56	n-Propyl acetate-M	C ₅ H ₁₀ O ₂	102.1	706.7	167.613	1.16446	Esters	101.31 ±	101.55 ±	86.60 ± 2.18e	139.08 ±	149.82 ± 3.98b	170.10 ±	98.83 ±	Monomer
								4.58d	4.20d		2.03c		5.97a	3.73d	
#61	Ethyl Acetate	C ₄ H ₈ O ₂	88.1	608.4	138.664	1.33719	Esters	983.29 ±	781.11 ±	1239.55 ±	4427.55 ±	4493.10 ±	2900.81 ±	661.58 ±	
								5.26d	10.65e	12.18c	46.08a	60.38a	125.47b	26.40f	
#66	Methyl acetate	C ₃ H ₆ O ₂	74.1	537	119.411	1.19298	Esters	2076.91 ±	3281.93 ±	3462.17 ±	3156.05 ±	2778.39 ±	2579.62 ±	2794.58 ±	
								41.91e	51.25b	82.82a	105.14b	20.20c	142.72d	150.64c	
#77	Methyl valerate	C ₆ H ₁₂ O ₂	116.2	825.4	221.138	1.564	Esters	184.58 ±	265.38 ±	229.94 ±	85.13 ±	112.33 ±	26.46 ±	22.74 ±	
								3.42c	11.24a	8.01b	4.75e	7.51d	2.25f	0.97f	
#84	Methyl butyrate-D	C ₅ H ₁₀ O ₂	102.1	715.5	171.206	1.42264	Esters	223.70 ±	223.49 ±	346.64 ±	724.64 ±	490.30 ± 8.65b	137.54 ±	124.28 ±	Dimer
								12.91d	8.60d	2.97c	12.16a		5.71e	7.93e	

#87	Methyl 3-methylbutanoate	C ₆ H ₁₂ O ₂	116.2	768.2	192.552	1.53234	Esters	47.29 ± 2.46e	72.17 ± 3.35c	81.77 ± 5.22b	131.89 ± 0.95a	60.74 ± 1.90d	9.83 ± 1.35f	11.66 ± 2.73f	Monomer
#88	Methyl butyrate-M	C ₅ H ₁₀ O ₂	102.1	717.2	171.868	1.15016	Esters	56.82 ± 3.08g	64.72 ± 2.38f	102.63 ± 1.25c	247.44 ± 3.64a	203.00 ± 2.20b	93.22 ± 4.79d	75.80 ± 3.47e	
#89	Butyl acetate-M	C ₆ H ₁₂ O ₂	116.2	803.5	209.421	1.23849	Esters	58.56 ± 1.11d	50.87 ± 1.15e	58.60 ± 0.93d	95.98 ± 1.46a	70.73 ± 4.66c	78.65 ± 2.04b	75.99 ± 1.71b	
#100	Butyl acetate-D	C ₆ H ₁₂ O ₂	116.2	802.5	208.857	1.61975	Esters	9.75 ± 0.12d	10.27 ± 0.69d	11.89 ± 0.61d	76.35 ± 2.10a	75.03 ± 2.69a	24.36 ± 0.50b	14.98 ± 0.59c	Dimer
#4	<i>trans</i> -Linalool oxide-M	C ₁₀ H ₁₈ O ₂	170.3	1084	471.749	1.2622	Heterocycle s	758.03 ± 44.00e	1825.64 ± 37.04c	2009.57 ± 68.25a	1874.56 ± 59.01bc	1956.22 ± 22.98ab	1316.65 ± 36.34d	1900.77 ± 54.92bc	Monomer
#5	<i>trans</i> -Linalool oxide-D	C ₁₀ H ₁₈ O ₂	170.3	1083.7	471.372	1.81672	Heterocycle s	161.61 ± 27.97d	702.53 ± 40.82b	961.05 ± 46.39a	661.56 ± 36.27b	680.84 ± 21.23b	297.56 ± 22.04c	672.22 ± 46.71b	
#6	2,3-Dimethyl-5-ethylpyrazine	C ₈ H ₁₂ N ₂	136.2	1069.3	450.642	1.23366	Heterocycle s	738.73 ± 33.66a	678.81 ± 25.98b	743.55 ± 16.90a	430.63 ± 15.39d	584.38 ± 31.71c	253.16 ± 29.35e	212.85 ± 10.48e	Monomer
#7	<i>cis</i> -Linalool Oxide-M	C ₁₀ H ₁₈ O ₂	170.3	1065.4	444.989	1.25948	Heterocycle s	300.43 ± 9.25d	810.65 ± 17.82ab	815.78 ± 26.51ab	793.01 ± 36.69ab	820.78 ± 10.40a	504.27 ± 23.63c	775.16 ± 18.81b	
#8	<i>cis</i> -Linalool Oxide-D	C ₁₀ H ₁₈ O ₂	170.3	1065.9	445.742	1.81129	Heterocycle s	56.73 ± 8.38f	207.18 ± 22.20b	230.27 ± 8.85a	132.15 ± 8.21d	153.79 ± 15.82c	56.70 ± 4.56f	92.27 ± 4.28e	
#17	2-Pentyl furan	C ₉ H ₁₄ O	138.2	993.1	343.037	1.25129	Heterocycle s	218.00 ± 5.89d	199.92 ± 4.88e	258.79 ± 4.33b	240.07 ± 5.53c	357.34 ± 11.77a	135.28 ± 4.67f	193.31 ± 3.43e	Monomer
#29	2-Acetylfuran	C ₆ H ₆ O ₂	110.1	907.9	270.326	1.11836	Heterocycle s	63.26 ± 3.84d	53.14 ± 2.94e	76.90 ± 3.80c	97.47 ± 7.49b	106.64 ± 2.30a	63.65 ± 1.18d	93.89 ± 4.24b	
#47	Furfural-M	C ₅ H ₄ O ₂	96.1	825.8	221.326	1.08524	Heterocycle s	79.21 ± 8.50b	53.94 ± 3.63c	68.96 ± 4.18b	50.83 ± 1.90c	56.60 ± 6.89c	71.28 ± 9.23b	489.96 ± 7.22a	
#48	Furfural-D	C ₅ H ₄ O ₂	96.1	824.7	220.75	1.33466	Heterocycle s	87.51 ± 8.64b	61.26 ± 3.44c	84.86 ± 4.07b	24.09 ± 3.65d	21.81 ± 1.82d	23.31 ± 1.38d	227.41 ± 3.07a	Dimer

#13	Methyl-5-hepten-2-one	C ₈ H ₁₄ O	126.2	990.2	340.586	1.17521	Ketones	4850.83 ± 184.15a	4906.21 ± 41.21a	3800.81 ± 71.72b	2077.25 ± 53.39d	2425.70 ± 42.15c	667.94 ± 27.70f	836.22 ± 27.87e	
#31	2-Heptanone-M	C ₇ H ₁₄ O	114.2	890.7	256.143	1.26224	Ketones	136.77 ± 4.75e	186.67 ± 1.85bc	154.40 ± 3.70d	156.16 ± 4.05d	182.35 ± 4.44c	200.17 ± 4.86a	190.94 ± 2.13b	
#35	2-Heptanone-D	C ₇ H ₁₄ O	114.2	887.4	254.37	1.62948	Ketones	274.99 ± 12.97c	409.58 ± 7.32a	358.34 ± 10.02b	105.49 ± 5.78e	206.92 ± 1.47d	36.60 ± 3.94g	75.86 ± 5.85f	Dimer
#39	Dihydro-2(3h)- furanone	C ₄ H ₆ O ₂	86.1	919.2	279.956	1.07948	Ketones	226.80 ± 27.33b	183.03 ± 5.67c	148.99 ± 5.12d	78.10 ± 5.98e	79.47 ± 7.04e	155.05 ± 10.81d	327.73 ± 1.80a	
#51	Mesityl oxide	C ₆ H ₁₀ O	98.1	790	202.166	1.44485	Ketones	3501.78 ± 32.03a	3520.86 ± 63.25a	2572.35 ± 46.44b	574.98 ± 6.25c	601.05 ± 6.19c	467.39 ± 3.43d	610.79 ± 13.40c	
#63	2-Butanone	C ₄ H ₈ O	72.1	583.6	131.984	1.24689	Ketones	3792.82 ± 29.72a	3812.36 ± 126.06a	3417.91 ± 38.76b	2691.36 ± 42.46c	2625.41 ± 14.11c	487.81 ± 23.00e	1900.21 ± 62.67d	
#71	3-Hydroxybutan-2-one	C ₄ H ₈ O ₂	88.1	711.8	169.704	1.05584	Ketones	102.06 ± 6.05c	104.29 ± 2.36c	101.43 ± 4.58c	42.49 ± 0.51e	53.84 ± 4.65d	163.49 ± 1.91b	233.85 ± 3.18a	
#73	(E)-3-Penten-2-one	C ₅ H ₈ O	84.1	737	179.92	1.09113	Ketones	47.88 ± 2.32b 0.39e	29.23 ± 0.39e	33.57 ± 0.78d	40.88 ± 0.25c	41.12 ± 2.24c	29.65 ± 0.71e	54.01 ± 1.30a	
#83	3-Pentanone	C ₅ H ₁₀ O	86.1	694.6	162.724	1.35332	Ketones	155.50 ± 5.27d	157.30 ± 4.08d	265.18 ± 3.34a	216.20 ± 3.25b	164.58 ± 4.48c	59.64 ± 1.98f	70.18 ± 1.30e	
#86	2-Hexanone	C ₆ H ₁₂ O	100.2	791.2	202.794	1.5026	Ketones	221.88 ± 15.77bc	235.16 ± 7.97ab	238.55 ± a	211.82 ± 4.25c	175.61 ± 7.22d	97.43 ± 3.72e	181.93 ± 9.11d	
#94	Acetone	C ₃ H ₆ O	58.1	488.6	106.359	1.11507	Ketones	10415.09 ± 113.11a	9632.76 ± 43.85b	8936.56 ± 20.67c	8070.92 ± 110.72d	7773.82 ± 33.39e	4016.98 ± 55.74g	5033.12 ± 148.60f	
#95	Cyclopentanone	C ₅ H ₈ O	84.1	785	199.494	1.33634	Ketones	137.55 ± 6.99b	123.94 ± 3.69c	116.32 ± 0.88c	101.32 ± 2.82d	101.24 ± 2.64d	175.35 ± 1.53a	123.95 ± 7.03c	
#99	2-Pentanone	C ₅ H ₁₀ O	86.1	689.3	160.591	1.37061	Ketones	91.89 ± 2.77a 6.97c	75.08 ± 6.97c	95.80 ± 0.64a	79.23 ± 0.65bc	83.79 ± 2.48b	47.60 ± 1.13d	17.14 ± 0.42e	

#80	Ethylsulfide	C ₄ H ₁₀ S	90.2	700.6	165.14	1.04444	Sulfides	231.00 ± 10.86a	153.32 ± 3.50c	130.14 ± 3.14de	191.50 ± 1.39b	232.92 ± 11.15a	119.99 ± 5.97e	137.28 ± 3.44d	
#9	γ-Terpinene	C ₁₀ H ₁₆	136.2	1051.8	425.39	1.22278	Terpenes	353.01 ± 7.87b	225.88 ± 8.28d	235.10 ± 12.31d	332.22 ± 2.38c	405.93 ± 17.93a	99.37 ± 5.61e	109.56 ± 3.89e	
#19	α-Phellandrene	C ₁₀ H ₁₆	136.2	1001.5	353.049	1.22014	Terpenes	29.67 ± 0.37e	36.61 ± 1.72d	46.45 ± 4.28c	72.89 ± 4.41b	89.94 ± 4.00a	42.13 ± 2.71cd	45.04 ± 4.16c	
#27	α-Fenchene	C ₁₀ H ₁₆	136.2	938.8	296.703	1.21853	Terpenes	59.41 ± 1.96d	70.89 ± 4.66c	60.06 ± 2.10d	124.36 ± 4.81b	176.55 ± 2.79a	49.30 ± 2.61e	35.89 ± 2.62f	
#10	1	/	/	1037.3	404.66	1.45519		314.09 ± 14.77a	244.12 ± 8.49c	229.29 ± 11.62c	280.79 ± 3.34b	300.53 ± 8.61a	183.80 ± 17.38d	167.19 ± 5.87d	Unidentified
#11	2	/	/	1026.9	389.584	1.24453		465.38 ± 11.92c	318.84 ± 4.35f	373.39 ± 2.17e	645.57 ± 12.63b	701.92 ± 14.75a	271.29 ± 4.71g	432.90 ± 16.84d	Unidentified
#16	3	/	/	986	336.956	1.76743		589.83 ± 5.59b	686.70 ± 1.13a	598.33 ± 8.05b	282.72 ± 6.15c	205.20 ± 15.82d	114.18 ± 7.83f	179.94 ± 3.81e	Unidentified
#18	4	/	/	999.1	349.637	1.20362		45.83 ± 3.21d	52.23 ± 0.93d	67.84 ± 8.37c	92.68 ± 11.12b	155.93 ± 3.96a	92.73 ± 6.27b	22.92 ± 1.80e	Unidentified
#28	5	/	/	927.8	287.347	1.19921		33.96 ± 3.38f	53.18 ± 1.01e	71.96 ± 2.65d	186.02 ± 2.74a	172.67 ± 3.43b	65.95 ± 3.93d	108.72 ± 5.65c	Unidentified
#30	6	/	/	895	259.334	1.14439		60.29 ± 1.51e	77.09 ± 2.34d	92.33 ± 3.45c	163.04 ± 8.29b	215.18 ± 3.93a	63.01 ± 3.00e	52.05 ± 2.63f	Unidentified
#34	7	/	/	899.2	262.88	1.60755		323.13 ± 13.35e	366.88 ± 2.42d	426.19 ± 9.05ab	433.80 ± 7.60ab	387.35 ± 16.34c	442.11 ± 2.67a	418.06 ± 3.21b	
#37	8	/	/	1041.7	410.973	1.20956		129.16 ± 30.02a	36.85 ± 6.58b	31.03 ± 5.18b	31.29 ± 1.41b	41.24 ± 2.75b	23.29 ± 0.97b	43.27 ± 6.28b	Unidentified
#38	9	/	/	914.4	275.848	1.41123		130.10 ± 19.63a	108.88 ± 4.90b	115.33 ± 2.68ab	41.00 ± 5.64c	39.01 ± 3.12c	51.29 ± 4.41c	103.58 ± 1.32b	Unidentified

#40	10	/	/	1007.5	361.799	1.82086	616.77 ± 58.86a	168.78 ± 12.37c	239.46 ± 18.12b	180.46 ± 7.76c	99.24 ± 1.58d	68.37 ± 11.82d	76.60 ± 10.89d	Unidentified
#41	11	/	/	1009.5	364.587	1.32981	1156.77 ± 12.26a	728.72 ± 2.16c	766.24 ± 32.58b	713.16 ± 8.36c	624.16 ± 26.96d	284.15 ± 23.29e	307.28 ± 9.58e	Unidentified
#43	12	/	/	920.8	281.311	1.59935	164.50 ± 3.37f	133.61 ± 2.25g	379.38 ± 2.47c	593.62 ± 10.19a	541.37 ± 4.26b	205.78 ± 15.79e	226.99 ± 6.70d	Unidentified
#54	13	/	/	732.5	178.089	1.33282	1051.63 ± 56.16a	642.44 ± 11.53c	716.12 ± 21.04b	319.85 ± 12.98e	434.40 ± 10.60d	106.52 ± 2.67g	196.63 ± 9.03f	Unidentified
#62	14	/	/	596	135.324	1.28903	1427.52 ± 8.44d	1025.42 ± 15.62e	1467.82 ± 4.50c	1889.59 ± 26.99a	1851.42 ± 4.07b	700.14 ± 13.98g	966.96 ± 30.87f	Unidentified
#65	15	/	/	528.3	117.054	1.23786	137.48 ± 1.33e	89.81 ± 1.85f	156.96 ± 2.74d	288.81 ± 3.42a	247.15 ± 0.62b	132.75 ± 6.45e	176.50 ± 15.75c	Unidentified
#67	16	/	/	740.4	181.295	1.42896	366.31 ± 9.00d	544.29 ± 2.68a	485.77 ± 7.42b	313.04 ± 8.74e	397.08 ± 5.92c	101.91 ± 6.50g	177.26 ± 6.85f	Unidentified
#69	17	/	/	739.4	180.902	1.15466	33.29 ± 2.67d	33.70 ± 1.78d	35.61 ± 2.05d	68.12 ± 2.96c	80.78 ± 3.09b	70.45 ± 5.57c	93.34 ± 1.58a	Unidentified
#70	18	/	/	808.2	211.942	1.1587	179.34 ± 5.14b	98.98 ± 5.12e	124.19 ± 1.20d	195.68 ± 2.38a	136.50 ± 2.91c	59.15 ± 2.78g	65.04 ± 1.51f	Unidentified
#72	19	/	/	734.1	178.741	1.07197	33.72 ± 2.87c	9.46 ± 1.45e	12.53 ± 1.24e	25.48 ± 2.56d	35.65 ± 0.94c	58.41 ± 1.31a	50.06 ± 2.16b	Unidentified
#74	20	/	/	805.1	210.264	1.04222	355.04 ± 18.51a	167.18 ± 3.92d	139.91 ± 2.05e	248.21 ± 4.30c	264.11 ± 5.60b	103.21 ± 5.21f	149.85 ± 5.93e	Unidentified
#75	21	/	/	810.3	213.051	1.48935	458.64 ± 11.23a	210.09 ± 10.62e	300.97 ± 2.61c	348.38 ± 10.58b	262.37 ± 9.19d	51.13 ± 2.51f	49.00 ± 2.16f	Unidentified
#85	22	/	/	767.4	192.24	1.47719	113.23 ± 4.55f	170.85 ± 3.18d	238.31 ± 4.23c	382.54 ± 13.92a	355.51 ± 7.00b	148.55 ± 4.50e	166.38 ± 11.87d	Unidentified

#90	23	/	/	827.4	222.218	1.26542	180.96 ±	202.27 ±	169.58 ±	143.22 ±	175.04 ±	88.37 ±	113.99 ±	Unidentified
							2.51b	6.06a	0.74c	4.28d	4.46bc	3.68f	4.27e	

Data were expressed as mean ± SD (n = 3).

MW represents molecular mass; RI represents relative retention index; Rt represents retention time; Dt represents relative migration time; The suffixe-M represents monomer of volatile components while the suffixe-D represents dimer. Values in a row followed by different letters are significantly different ($p < 0.05$).

Table S3 Characterization and contents of the volatile compounds of sweet and floral aroma black tea during the entire manufacturing process based on GC-MS.

No.	Compounds	R ^t ^a	RI ^b	RI ^c	ID	Compound types	Contents (µg/L)							VIP	Significance
							Fresh	Witherin	Shakin	Rollin	Fermentatio	First	Final		
							leaves	g	g	g	n	drying	firing		
7	2-Methylbutanol	10.73	711	718	MS, RI	Alcohols	0.11 ±	0.32 ±	0.12 ±	0.02 ±	0.03 ± 0.00c	0.02 ±	0.01 ±	0.96	0
							0.02b	0.06a	0.03b	0.00c		0.00c	0.00c		
10	(Z)-2-Pentenol	11.85	747	746	MS, RI	Alcohols	0.73 ±	2.41 ±	2.20 ±	1.41 ±	1.93 ±	1.66 ±	1.14 ±	1.16	0
							0.08e	0.42a	0.66ab	0.08cd		0.30bcd	0.10de		
14	(E)-3-Hexen-1-ol	14.9	844	855	MS, RI	Alcohols	43.06 ±	31.88 ±	26.14 ±	12.79 ±	12.10 ± 1.72c	8.13 ±	6.24 ±	0.98	0
							4.70a	4.15b	8.15b	1.81c		1.85c	0.42c		
15	1-Hexanol	15.28	856	858	MS, RI	Alcohols	6.85 ±	5.11 ±	3.99 ±	1.91 ±	1.82 ± 0.26c	1.31 ±	0.93 ±	0.95	0
							0.79a	0.23b	1.84b	0.18c		0.28c	0.14c		
19	2-Heptanol	16.43	893	888	MS, RI	Alcohols	1.47 ±	4.88 ±	0.44 ±	0.34 ±	0.45 ± 0.05b	0.37 ±	0.31 ±	0.98	0.029
							0.79b	4.13a	0.18b	0.05b		0.08b	0.02b		
23	1-Heptanol	19.11	975	970	MS, RI	Alcohols	4.21 ±	2.84 ±	0.86 ±	0.35 ±	0.34 ± 0.06d	0.28 ±	0.24 ±	0.96	0
							0.58a	0.08b	0.13c	0.04d		0.07d	0.04d		
24	1-Octen-3-ol	19.49	986	981	MS, RI	Alcohols	7.36 ±	12.51 ±	4.60 ±	1.93 ±	2.31 ± 0.46c	1.96 ±	1.28 ±	0.90	0
							1.50b	4.19a	1.07bc	0.22c		0.62c	0.08c		
33	2-Ethyl-1-hexanol	21.36	1031	1039	MS, RI	Alcohols	1.09 ±	1.78 ±	0.74 ±	0.34 ±	0.34 ± 0.06c	0.34 ±	0.22 ±	0.88	0
							0.06b	0.69a	0.14bc	0.03c		0.11c	0.03c		
37	2-Methyl-6-methylene-3,7-octadien-2-ol	21.57	1037	/	MS, RI	Alcohols	7.15 ±	8.04 ±	4.00 ±	1.09 ±	1.63 ± 0.41c	0.91 ±	1.17 ±	0.85	0
							1.30a	2.27a	0.85b	0.05c		0.32c	0.25c		

39	Benzyl alcohol	21.79	1044	1051	MS, RI	Alcohols	46.34 ± 14.84ab	48.67 ± 13.83a	33.61 ± 4.60b	6.81 ± 0.27c	7.94 ± 1.89c	5.13 ± 1.55c	6.32 ± 1.21c	0.86	0
48	Linalool	24.17	1111	1112	MS, RI	Alcohols	141.23 ± 12.82b	210.87 ± 53.68a	109.38 ± 23.19b	47.01 ± 5.73c	45.98 ± 7.98c	37.29 ± 12.64c	31.93 ± 2.08c	0.85	0
49	3,7-Dimethyl-1,5,7-octatriene-3-ol (Hotrienol)	24.17	1111	1106	MS, RI	Alcohols	163.46 ± 15.09b	245.50 ± 62.60a	91.32 ± 77.57bc	39.17 ± 32.13c d	35.81 ± 28.66cd	2.54 ± 0.94d	3.85 ± 1.03d	0.84	0
51	Phenylethyl alcohol	24.7	1126	1127	MS, RI	Alcohols	52.58 ± 6.42a	58.93 ± 16.62a	53.43 ± 9.01a	14.94 ± 0.62b	16.36 ± 4.14b	11.96 ± 3.69b	13.84 ± 2.73b	0.89	0
55	1-Dodecanol	25.17	1140	1470	MS, RI	Alcohols	1.16 ± 0.16b	1.90 ± 0.27a	0.69 ± 0.20c	0.09 ± 0.01d	0.14 ± 0.04d	0.06 ± 0.02d	0.05 ± 0.01d	0.88	0
60	1-Nonanol	26.36	1173	1176	MS, RI	Alcohols	6.72 ± 0.67a	4.60 ± 0.94b	1.94 ± 0.20c	0.64 ± 0.08d	0.61 ± 0.12d	0.49 ± 0.25d	0.37 ± 0.06d	0.95	0
68	α-Terpineol	27.36	1201	1202	MS, RI	Alcohols	2.01 ± 0.25b	2.93 ± 0.45a	1.91 ± 0.34b	0.88 ± 0.05c	0.94 ± 0.19c	0.75 ± 0.24c	0.66 ± 0.05c	0.86	0
74	7-Methyl-3-methylene-6-octen-1-ol	28.02	1223	1221	MS, RI	Alcohols	3.24 ± 0.29b	4.59 ± 0.29a	2.69 ± 0.50c	1.26 ± 0.16d	1.42 ± 0.29d	1.14 ± 0.34d	0.92 ± 0.09d	0.86	0
102	α-Nerolidol	37.66	1572	1566	MS, RI	Alcohols	1.31 ± 0.15ab	1.67 ± 0.59a	1.71 ± 0.41a	1.03 ± 0.09bc	1.04 ± 0.26bc	0.68 ± 0.28c	0.69 ± 0.04c	0.96	0.005
2	2-Methylpropanal	6.23	567	558	MS, RI	Aldehydes	0.08 ± 0.02d	0.76 ± 0.31b	1.23 ± 0.25a	0.44 ± 0.05c	0.64 ± 0.11bc	0.90 ± 0.15b	0.72 ± 0.04bc	1.21	0
4	3-Methylbutanal	8.18	630	634	MS, RI	Aldehydes	0.12 ± 0.04d	0.99 ± 0.37c	1.86 ± 0.27a	1.08 ± 0.11bc	1.79 ± 0.37a	1.84 ± 0.29a	1.49 ± 0.13ab	1.04	0
5	2-Methylbutanal	8.45	638	645	MS, RI	Aldehydes	0.25 ± 0.08e	3.43 ± 1.58bcd	5.93 ± 0.96a	2.06 ± 0.14d	3.06 ± 0.58cd	4.81 ± 0.86ab	4.34 ± 0.08bc	1.28	0

11	Hexanal	12.86	779	782	MS, RI	Aldehydes	2.49 ± 0.49c	7.96 ± 3.89a	3.63 ± 0.29bc	4.08 ± 0.55bc	7.94 ± 1.92a	6.82 ± 1.86ab	2.30 ± 0.23c	1.28	0.004
12	2-Ethyl-2-butenal	14.06	817	808	MS, RI	Aldehydes	0.37 ± 0.08b	1.06 ± 0.24b	0.25 ± 0.11b	1.81 ± 2.71b	6.06 ± 1.08a	0.29 ± 0.08b	0.41 ± 0.59b	1.43	0
13	(E)-2-Hexenal	14.9	844	850	MS, RI	Aldehydes	16.43 ± 1.71b	4.39 ± 2.06d	8.02 ± 0.94c	16.11 ± 0.11b	19.60 ± 3.16a	6.94 ± 1.30cd	3.90 ± 0.41d	1.76	0
21	Heptanal	16.52	899	903	MS, RI	Aldehydes	0.70 ± 0.13cd	1.87 ± 0.69a	0.76 ± 0.11bcd	1.04 ± 0.13bc d	1.35 ± 0.30ab	1.17 ± 0.42bc	0.46 ± 0.06d	1.29	0.003
22	Benzaldehyde	19	972	966	MS, RI	Aldehydes	70.81 ± 6.59a	71.39 ± 7.70a	26.65 ± 5.42b	6.83 ± 0.37c	10.36 ± 2.42c	6.52 ± 1.45c	6.32 ± 0.46c	0.88	0
31	Octanal	20.55	1008	1009	MS, RI	Aldehydes	0.55 ± 0.09a	0.64 ± 0.14a	0.25 ± 0.03b	0.18 ± 0.04b	0.20 ± 0.05b	0.23 ± 0.07b	0.14 ± 0.05b	0.91	0
66	Decanal	27.3	1199	1202	MS, RI	Aldehydes	13.37 ± 0.26a	8.49 ± 7.08ab	6.08 ± 2.08b	0.33 ± 0.01c	0.20 ± 0.06c	0.21 ± 0.04c	4.07 ± 0.64bc	1.00	0
71	β-Cyclocitral	27.55	1207	1210	MS, RI	Aldehydes	69.21 ± 3.21b	121.19 ± 3.08a	125.74 ± 26.97a	52.26 ± 4.25bc	67.02 ± 13.77b	33.52 ± 13.43cd	28.75 ± 3.19d	1.01	0
72	Safranal	27.69	1211	1201	MS, RI	Aldehydes	0.11 ± 0.01c	0.15 ± 0.01b	0.11 ± 0.02c	0.05 ± 0.00e	0.06 ± 0.01de	0.08 ± 0.02cd	0.21 ± 0.02a	1.68	0
75	2-Methyl-5-isopropenyl-1-cyclopenten-1-carboxaldehyde	28.17	1228	1271	MS, RI	Aldehydes	0.51 ± 0.03b	1.03 ± 0.20a	0.91 ± 0.17a	0.37 ± 0.03bc	0.36 ± 0.06bc	0.20 ± 0.05c	0.18 ± 0.04c	0.94	0
79	β-Citral	29.3	1266	1255	MS, RI	Aldehydes	383.03 ± 97.69bc	607.54 ± 162.77a	427.69 ± 77.19b	± 25.75c d	291.93 ± 55.99bcd	232.73 ± 68.83cd	186.95 ± 10.31d	0.89	0

81	Citral	29.73	1280	1276	MS, RI	Aldehydes	282.82 ± 243.33b	685.14 ± 81.48a	26.26 ± 4.71c	17.29 ± 1.31c	19.82 ± 4.29c	106.03 ± 165.72b c	66.47 ± 97.35bc	1.08	0
89	2-Butyl-2-octenal	32.69	1379	1378	MS, RI	Aldehydes	0.61 ± 0.09b	1.19 ± 0.35a	0.70 ± 0.15b	0.04 ± 0.00c	0.05 ± 0.01c	0.02 ± 0.01c	0.04 ± 0.02c	0.88	0
29	2,2,4,6,6-Pentamethylheptane	20.05	1002	995	MS, RI	Alkanes	17.91 ± 2.63a	11.98 ± 7.42b	6.40 ± 2.18c	0.30 ± 0.03d	0.42 ± 0.07d	0.80 ± 0.59d	0.09 ± 0.02d	0.92	0
30	Decane	20.26	1000	1000	MS, RI	Alkanes	3.94 ± 0.28a	3.19 ± 1.93a	1.72 ± 0.66b	0.14 ± 0.02c	0.14 ± 0.04c	0.19 ± 0.13c	0.12 ± 0.04c	0.88	0
35	2,2,4,4-Tetramethyloctane	21.48	1035	/	MS, RI	Alkanes	4.54 ± 0.68a	2.89 ± 1.83b	1.79 ± 0.55b	0.06 ± 0.01c	0.08 ± 0.02c	0.19 ± 0.15c	0.15 ± 0.13c	0.94	0
56	5-Ethyldecane	25.46	1148	1146	MS, RI	Alkanes	1.67 ± 0.31a	0.97 ± 0.72b	0.59 ± 0.21bc	0.02 ± 0.01c	0.02 ± 0.01c	0.05 ± 0.03c	0.04 ± 0.00c	0.95	0
58	5-Methylundecane	26.1	1166	1156	MS, RI	Alkanes	0.62 ± 0.18a	0.69 ± 0.45a	0.41 ± 0.12ab	0.11 ± 0.00b	0.13 ± 0.03b	0.09 ± 0.04b	0.06 ± 0.00b	0.82	0.003
59	3-Methylundecane	26.34	1173	1173	MS, RI	Alkanes	7.96 ± 0.70a	4.91 ± 2.98b	2.88 ± 0.87b	0.23 ± 0.01c	0.27 ± 0.06c	0.31 ± 0.20c	0.14 ± 0.03c	0.94	0
65	Dodecane	27.3	1199	1200	MS, RI	Alkanes	13.32 ± 0.24a	8.87 ± 6.47ab	6.09 ± 2.11b	0.19 ± 0.02c	0.20 ± 0.06c	0.41 ± 0.29c	0.06 ± 0.00c	0.92	0
92	Tetradecane	33.26	1398	1400	MS, RI	Alkanes	5.23 ± 0.51ab	4.33 ± 1.99ab	2.92 ± 0.82b	7.00 ± 0.01a	6.94 ± 0.05a	4.75 ± 3.77ab	7.02 ± 0.03a	0.80	0.052
101	3-Methylpentadecane	37.66	1572	1574	MS, RI	Alkanes	1.67 ± 0.26a	1.61 ± 0.46a	1.08 ± 0.21b	0.17 ± 0.02c	0.13 ± 0.02c	0.12 ± 0.06c	0.08 ± 0.01c	0.87	0
104	Hexadecane	38.35	1599	1600	MS, RI	Alkanes	1.16 ± 0.08ab	1.25 ± 0.27a	0.96 ± 0.19b	0.22 ± 0.02c	0.17 ± 0.01c	0.12 ± 0.04c	0.08 ± 0.01c	0.87	0

18	1,3,5,7-Cyclooctatetraene	16.23	887	880	MS, RI	Alkenes	0.60 ± 0.08a	0.70 ± 0.09a	0.40 ± 0.07b	0.23 ± 0.02c	0.24 ± 0.05c	0.16 ± 0.04c	0.19 ± 0.05c	0.85	0
27	α -Phellandrene	20.03	993	1005	MS, RI	Alkenes	88.11 ± 6.13b	130.62 ± 29.86a	73.10 ± 13.87b	36.42 ± 4.74c	38.41 ± 7.11c	30.78 ± 7.67c	28.00 ± 4.41c	0.86	0
28	β -Myrcene	20.03	1002	1007	MS, RI	Alkenes	88.16 ± 6.11b	130.90 ± 29.53a	73.13 ± 13.92b	36.41 ± 4.75c	38.48 ± 7.17c	30.78 ± 7.67c	28.02 ± 4.41c	0.86	0
32	δ -Carene	21.11	1024	1017	MS, RI	Alkenes	2.62 ± 0.22b	3.29 ± 0.55a	1.85 ± 0.37c	0.76 ± 0.11d	0.83 ± 0.16d	0.63 ± 0.17d	0.53 ± 0.09d	0.85	0
36	D-Limonene	21.57	1037	1038	MS, RI	Alkenes	16.94 ± 0.76b	20.27 ± 3.84a	10.56 ± 2.13c	4.61 ± 0.62d	4.94 ± 0.99d	3.74 ± 1.05d	3.01 ± 0.55d	0.85	0
40	β -Ocimene	22.13	1053	1053	MS, RI	Alkenes	29.72 ± 3.09b	40.40 ± 6.50a	24.50 ± 4.64b	11.58 ± 1.50c	12.72 ± 2.39c	9.62 ± 2.59c	9.10 ± 1.25c	0.85	0
42	β -Terpinene	22.64	1068	1056	MS, RI	Alkenes	11.98 ± 18.23bc	40.39 ± 6.49a	24.50 ± 4.64b	11.57 ± 1.50bc	12.71 ± 2.38bc	9.61 ± 2.59c	9.10 ± 1.25c	0.96	0.002
52	(E, E)-2,6-dimethyl-1,3,5,7-octatetraene	24.81	1129	1130	MS, RI	Alkenes	0.77 ± 0.04b	0.92 ± 0.10a	0.59 ± 0.11c	0.25 ± 0.03d	0.26 ± 0.05d	0.21 ± 0.06d	0.21 ± 0.03d	0.85	0
53	(E, Z)-2,6-dimethylocta-2,4,6-triene	25.02	1135	1131	MS, RI	Alkenes	8.74 ± 0.45b	12.03 ± 2.77a	6.41 ± 1.21c	3.00 ± 0.40d	3.10 ± 0.53d	2.37 ± 0.58d	2.03 ± 0.38d	0.85	0
54	1,3,8-p-Menthatriene	25.15	1139	1127	MS, RI	Alkenes	2.67 ± 0.11b	3.40 ± 0.51a	2.16 ± 0.38c	0.97 ± 0.12d	1.02 ± 0.19d	0.80 ± 0.20d	0.78 ± 0.13d	0.84	0
63	1-Dodecene	27.05	1193	1192	MS, RI	Alkenes	0.93 ± 0.05b	0.94 ± 0.39b	2.56 ± 1.53a	0.70 ± 0.03b	0.61 ± 0.10b	0.51 ± 0.17b	0.67 ± 0.35b	1.14	0.015
69	(E)-3-Dodecene	27.46	1204	1185	MS, RI	Alkenes	0.22 ± 0.01a	0.20 ± 0.10ab	0.13 ± 0.03abc	0.02 ± 0.00d	0.11 ± 0.08bcd	0.02 ± 0.01cd	0.06 ± 0.07cd	0.89	0.003
78	4,5-Dimethyl-2,6-octadiene	29.3	1266	/	MS, RI	Alkenes	383.24 ± 98.38bc	608.81 ± 163.21a	428.08 ± 76.63b	257.80 ±	237.34 ± 8.84cd	233.26 ± 69.05cd	187.08 ± 10.14d	0.87	0

										25.96c					
										d					
88	α -Cubebene	32.26	1365	1360	MS, RI	Alkenes	0.58 ± 0.25b	0.83 ± 0.12a	0.88 ± 0.17a	0.38 ± 0.02b	0.43 ± 0.13b	0.36 ± 0.15b	0.32 ± 0.03b	0.95	0.001
95	Caryophyllene	34.45	1446	1438	MS, RI	Alkenes	0.45 ± 0.05bc	1.15 ± 0.62a	0.85 ± 0.15ab	0.07 ± 0.01c	0.66 ± 0.13b	0.06 ± 0.04c	0.11 ± 0.02c	0.91	0
98	(Z)-Calamenene	37.02	1547	1546	MS, RI	Alkenes	4.02 ± 0.57a	4.19 ± 0.76a	3.50 ± 0.62a	1.13 ± 0.06b	1.18 ± 0.31b	0.99 ± 0.42b	1.26 ± 0.17b	0.89	0
100	β -Calacorene	37.57	1568	1566	MS, RI	Alkenes	0.76 ± 0.16a	0.77 ± 0.19a	0.64 ± 0.11a	0.21 ± 0.01b	0.23 ± 0.06b	0.20 ± 0.10b	0.38 ± 0.06b	0.94	0
105	Cadalene	40.74	1670	1674	MS, RI	Alkenes	0.38 ± 0.06b	0.57 ± 0.07a	0.37 ± 0.05b	0.13 ± 0.01c	0.13 ± 0.02c	0.09 ± 0.03c	0.13 ± 0.03c	0.88	0
80	Caprolactam	29.53	1273	1266	MS, RI	Amines	0.16 ± 0.02b	0.57 ± 0.52a	0.23 ± 0.04ab	0.12 ± 0.04b	0.25 ± 0.05ab	0.19 ± 0.03ab	0.11 ± 0.12b	0.95	0.169
9	Toluene	11.76	744	760	MS, RI	Aromatic hydrocarbons	1.17 ± 0.22b	1.75 ± 0.08a	0.98 ± 0.22b	0.42 ± 0.09c	0.57 ± 0.16c	0.62 ± 0.12c	0.60 ± 0.08c	0.91	0
16	1,3-Dimethylbenzene(m-xylene)	15.43	861	866	MS, RI	Aromatic hydrocarbons	0.92 ± 0.05a	1.00 ± 0.06a	0.52 ± 0.12b	0.24 ± 0.03c	0.25 ± 0.05c	0.19 ± 0.06c	0.17 ± 0.03c	0.86	0
34	o-Cymene	21.4	1032	1039	MS, RI	Aromatic hydrocarbons	14.66 ± 0.53a	16.27 ± 3.83a	7.63 ± 1.65b	3.21 ± 0.39c	3.15 ± 0.55c	2.62 ± 0.63c	1.94 ± 0.39c	0.86	0
47	1,2-Dimethyl-4-vinylbenzene	23.79	1100	1100	MS, RI	Aromatic hydrocarbons	3.54 ± 0.41a	4.14 ± 0.93a	2.20 ± 0.46b	0.94 ± 0.10c	0.93 ± 0.16c	0.71 ± 0.19c	0.57 ± 0.08c	0.84	0

41	(Z)-3-Hexenyl crotonate	22.36	1060	/	MS, RI	Esters	0.41 ± 0.08b	0.61 ± 0.10a	0.37 ± 0.07b	0.22 ± 0.03c	0.25 ± 0.04c	0.16 ± 0.05c	0.14 ± 0.01c	0.89	0
43	Formic acid, octyl ester	22.93	1076	1109	MS, RI	Esters	2.78 ± 0.36a	2.53 ± 0.12a	1.20 ± 0.23b	0.53 ± 0.08c	0.58 ± 0.12c	0.53 ± 0.17c	0.49 ± 0.11c	0.90	0
62	(E)-3-Hexenyl butanoate	26.9	1189	1185	MS, RI	Esters	23.62 ± 4.13b	30.98 ± 5.30b	43.82 ± 12.78a	15.38 ± 1.28cd	12.61 ± 3.51d	7.88 ± 3.34d	7.13 ± 1.16d	1.09	0
64	Octanoic acid, ethyl ester	27.19	1197	1197	MS, RI	Esters	1.10 ± 0.22a	1.11 ± 0.32a	1.35 ± 0.25a	0.18 ± 0.02b	0.20 ± 0.04b	0.16 ± 0.04b	0.18 ± 0.04b	0.97	0
67	(E)-2-Hexenyl butanoate	27.3	1200	1195	MS, RI	Esters	8.92 ± 0.21a	1.77 ± 0.59c	4.03 ± 2.22b	1.30 ± 0.05c	1.00 ± 0.31c	0.64 ± 0.28c	0.65 ± 0.25c	1.22	0
70	Methyl salicylate	27.55	1207	1206	MS, RI	Esters	126.18 ± 5.75b	218.76 ± 4.46a	220.82 ± 46.80a	93.92 ± 7.76bc	119.58 ± 24.33b	61.99 ± 24.16c	53.49 ± 5.73c	1.00	0
73	Bis(2-ethylhexyl) carbonate	27.75	1214	/	MS, RI	Esters	0.46 ± 0.07a	0.25 ± 0.14b	0.20 ± 0.06b	0.13 ± 0.03bc	0.13 ± 0.04bc	0.06 ± 0.07c	0.02 ± 0.00c	1.08	0
76	(Z)-3-Hexenyl pentanoate	28.36	1234	1235	MS, RI	Esters	4.58 ± 0.58b	7.62 ± 1.01b	23.12 ± 6.17a	7.83 ± 0.47b	6.82 ± 1.84b	5.76 ± 2.46b	6.90 ± 1.04b	1.30	0
82	Ethyl salicylate	29.88	1285	1286	MS, RI	Esters	0.47 ± 0.15c	1.47 ± 0.72b	3.63 ± 0.25a	0.40 ± 0.05c	0.63 ± 0.15c	0.15 ± 0.04c	0.13 ± 0.05c	1.18	0
83	3,7-Dimethyl-cis-2,6-octadienyl formate	30.56	1308	1282	MS, RI	Esters	1.36 ± 0.28b	5.74 ± 4.64a	3.21 ± 0.89ab	2.83 ± 0.05ab	3.70 ± 0.87ab	1.13 ± 0.52b	1.12 ± 0.16b	1.02	0.067
85	(E)-Methyl 3,7-dimethylocta-2,6-dienoate	31.19	1329	1321	MS, RI	Esters	5.98 ± 0.94c	12.29 ± 1.39b	18.51 ± 3.98a	6.52 ± 0.21c	5.83 ± 1.33c	3.45 ± 1.20c	4.51 ± 0.59c	1.13	0
86	Dimethyl salicylate	31.71	1346	1347	MS, RI	Esters	0.20 ± 0.06ab	0.17 ± 0.10b	0.34 ± 0.18a	0.15 ± 0.05b	0.17 ± 0.04b	0.09 ± 0.04b	0.10 ± 0.01b	1.16	0.052
90	(Z)-3-Hexenyl hexanoate	32.77	1382	1381	MS, RI	Esters	13.89 ± 4.99b	16.29 ± 4.67b	50.99 ± 13.58a	19.55 ± 1.61b	16.99 ± 4.45b	11.55 ± 5.84b	15.82 ± 5.15b	1.30	0

91	(Z)-3-Hexenyl (Z)-3-hexenoate	32.91	1387	1388	MS, RI	Esters	3.78 ± 0.58b	4.06 ± 0.48b	4.42 ± 1.12b	1.58 ± 0.18b	1.27 ± 0.30b	0.76 ± 0.32b	9.15 ± 6.42a	1.31	0.015
99	(R)-4,4,7a-Trimethyl-5,6,7,7a-tetrahydrobenzofuran-2(4H)-one (Dihydroactinidiolide)	37.42	1562	1548	MS, RI	Esters	0.80 ± 0.11bc	1.29 ± 0.32a	0.99 ± 0.17b	0.46 ± 0.04de	0.56 ± 0.14cd	0.25 ± 0.10e	0.26 ± 0.09e	0.91	0
103	(Z)-3-Hexenyl benzoate	38	1585	1575	MS, RI	Esters	0.11 ± 0.01c	0.29 ± 0.04c	1.30 ± 0.24a	1.14 ± 0.08a	1.26 ± 0.25a	0.80 ± 0.28b	0.81 ± 0.09b	1.15	0
6	2-Ethylfuran	9.49	671	684	MS, RI	Heterocycli c compounds	6.09 ± 2.25a	4.48 ± 0.39a	2.57 ± 0.81b	1.06 ± 0.02b	1.19 ± 0.24b	1.37 ± 0.47b	0.97 ± 0.08b	0.93	0
26	(E)-2-(1-Pentenyl)furan	20.03	993	1000	MS, RI	Heterocycli c compounds	9.65 ± 0.64ab	10.35 ± 8.72a	2.48 ± 3.40c	3.77 ± 0.50ab c	4.00 ± 0.75abc	3.20 ± 0.82bc	2.03 ± 1.68c	0.94	0.06
38	Pyrazine	21.72	1041	747	MS, RI	Heterocycli c compounds	2.07 ± 0.63c	4.12 ± 0.88a	3.08 ± 0.51b	1.01 ± 0.08d	1.15 ± 0.24d	0.83 ± 0.23d	0.86 ± 0.12d	0.91	0
45	Linalool oxide	23.17	1083	1092	MS, RI	Heterocycli c compounds	9.64 ± 0.49b	21.20 ± 5.19a	11.39 ± 1.94b	5.17 ± 0.91c	5.44 ± 1.20c	4.48 ± 1.31c	3.30 ± 0.22c	0.93	0
61	cis-Linalool oxide (pyranoid)	26.67	1182	1183	MS, RI	Heterocycli c compounds	5.29 ± 0.26b	9.18 ± 2.23a	6.81 ± 1.50b	1.95 ± 0.24c	2.52 ± 0.62c	2.21 ± 0.67c	2.19 ± 0.21c	0.90	0
77	Quinoline	29.04	1257	1242	MS, RI	Heterocycli c compounds	0.26 ± 0.02b	0.35 ± 0.03a	0.27 ± 0.06b	0.11 ± 0.01c	0.11 ± 0.02c	0.08 ± 0.03c	0.07 ± 0.01c	0.86	0

84	Indole	30.61	1310	1303	MS, RI	Heterocycli	10.86 ±	1.33 ±	0.24 ±	0.10 ±	0.09 ± 0.02b	0.05 ±	0.03 ±	1.17	0
						c compounds	1.66a	0.92b	0.03b	0.02b		0.02b	0.00b		
106	Caffeine	44.43	1788	1784	MS, RI	Heterocycli	0.61 ±	1.43 ±	1.42 ±	1.24 ±	1.57 ± 0.59a	1.19 ±	0.70 ±	1.16	0.13
						c compounds	0.08b	0.75ab	0.25ab	0.11ab		0.65ab	0.12ab		
8	3-Penten-2-one	10.84	714	714	MS, RI	Ketones	0.40 ±	0.38 ±	0.17 ±	0.07 ±	0.11 ± 0.02bc	0.11 ±	0.07 ±	0.89	0
							0.06a	0.08a	0.05b	0.01c		0.02bc	0.01c		
17	2-Heptanone	16.11	883	889	MS, RI	Ketones	1.01 ±	2.09 ±	0.61 ±	0.18 ±	0.26 ± 0.05cd	0.36 ±	0.36 ±	1.02	0
							0.13b	0.51a	0.17c	0.03d		0.09cd	0.05cd		
20	5-Hexen-3-one	16.43	893	/	MS, RI	Ketones	0.08 ±	0.26 ±	0.03 ±	0.02 ±	0.03 ± 0.01b	0.02 ±	0.01 ±	0.97	0.032
							0.04b	0.22a	0.01b	0.00b		0.01b	0.00b		
25	6-Methyl-5-hepten-2-one	19.82	996	988	MS, RI	Ketones	1.82 ±	2.80 ±	0.89 ±	0.38 ±	0.42 ± 0.08cd	0.25 ±	0.24 ±	0.90	0
							0.28b	0.62a	0.21c	0.03d		0.07d	0.01d		
44	3,5-Octadien-2-one	22.97	1077	1090	MS, RI	Ketones	13.30 ±	21.30 ±	14.64 ±	6.67 ±	11.32 ± 2.23b	5.22 ±	1.81 ±	0.99	0
							1.78b	0.36a	3.53b	0.11c		1.86c	0.18d		
46	3-Nonanone	23.5	1092	1089	MS, RI	Ketones	0.17 ±	0.23 ±	0.13 ±	0.03 ±	0.03 ± 0.01de	0.06 ±	0.02 ±	0.85	0
							0.02b	0.02a	0.04c	0.00de		0.02d	0.00e		
50	2,3,4-Trimethyl-2-cyclopenten-1-one	24.17	1111	1089	MS, RI	Ketones	5.31 ±	10.31 ±	0.86 ±	0.30 ±	0.35 ± 0.07a	1.80 ±	0.27 ±	0.79	0.487
							7.83a	15.66a	0.19a	0.01a		2.79a	0.04a		
57	5-Ethyl-6-methyl-3(E)-hepten-2-one	25.66	1153	1143	MS, RI	Ketones	1.04 ±	2.15 ±	1.02 ±	0.25 ±	0.33 ± 0.10c	0.33 ±	0.29 ±	0.92	0
							0.10b	0.52a	0.24b	0.04c		0.12c	0.07c		
93	(Z)-Jasmone	33.61	1413	1405	MS, RI	Ketones	5.61 ±	3.68 ±	2.01 ±	0.93 ±	0.98 ± 0.19d	0.56 ±	0.53 ±	0.98	0
							0.97a	0.77b	0.18c	0.04d		0.20d	0.08d		
94	α -Ionone	34.37	1443	1438	MS, RI	Ketones	1.19 ±	2.07 ±	1.34 ±	0.67 ±	0.82 ± 0.16cd	0.36 ±	0.31 ±	0.91	0
							0.23bc	0.41a	0.27b	0.04de		0.12e	0.05e		

96	Geranyl acetone	34.8	1460	1453	MS, RI	Ketones	0.43 ± 0.04b	0.74 ± 0.02a	0.62 ± 0.11a	0.40 ± 0.01b	0.44 ± 0.10b	0.15 ± 0.05c	0.14 ± 0.11c	1.06	0
97	β -Ionone	35.93	1504	1505	MS, RI	Ketones	8.95 ± 1.31bc	17.60 ± 2.78a	11.37 ± 2.29b	6.31 ± 0.18cd	7.80 ± 1.64c	4.10 ± 1.60d	3.80 ± 0.77d	0.94	0
3	Acetic acid	7.22	599	600	MS, RI	Organic acids	0.82 ± 0.08a	0.76 ± 0.26a	0.66 ± 0.08a	0.13 ± 0.02b	0.06 ± 0.09b	0.15 ± 0.04b	0.19 ± 0.05b	0.94	0
87	Geranic acid	31.9	1353	1355	MS, RI	Organic acids	1.36 ± 0.07b	2.25 ± 0.61b	10.15 ± 3.26a	2.69 ± 1.06b	3.57 ± 0.82b	1.66 ± 0.90b	2.05 ± 0.55b	1.28	0
1	Dimethyl sulfide	5.77	552	550	MS, RI	Sulfur compounds	1.56 ± 0.40c	13.26 ± 1.28a	12.74 ± 3.00a	5.37 ± 0.85b	6.60 ± 1.23b	4.85 ± 1.60b	2.22 ± 0.23c	1.11	0

Data were expressed as mean \pm SD (n = 3).

RT^a represents retention time; RI^b represents the linear retention indices calculated from a series of *n*-alkanes (C7-C40); RI^c represents retention indices referred to the literature value with HP-5ms column or equivalent chromatographic column [NIST Chemistry WebBook (<http://webbook.nist.gov/chemistry/>) and <http://www.flavornet.org/flavornet.html/>]. ID represents identification method. MS represents identification based on the NIST 11 database. VIP represents variable importance in the projection. Values in a row followed by different letters are significantly different ($p < 0.05$).

Table S4 The screened volatile components with rOAVs greater than one in sweet and floral aroma black tea during the entire manufacturing process.

Compounds	Threshold	Contents (µg/L)							rOAVs						
	values (µg/L)	Fresh leaves	Withering	Shaking	Rolling	Fermentation	First drying	Final firing	Fresh leaves	Withering	Shaking	Rolling	Fermentation	First drying	Final firing
Dimethyl sulfide	0.3	1.56	13.26	12.74	5.37	6.60	4.85	2.22	5.20	44.19	42.47	17.91	21.99	16.16	7.40
2-Methylpropanal	0.49	0.08	0.76	1.23	0.44	0.64	0.90	0.72	0.16	1.55	2.51	0.89	1.30	1.84	1.46
3-Methylbutanal	0.2	0.12	0.99	1.86	1.08	1.79	1.84	1.49	0.58	4.93	9.30	5.38	8.95	9.20	7.43
2-Methylbutanal	1	0.25	3.43	5.93	2.06	3.06	4.81	4.34	0.25	3.43	5.93	2.06	3.06	4.81	4.34
2-Ethylfuran	2.3	6.09	4.48	2.57	1.06	1.19	1.37	0.97	2.65	1.95	1.12	0.46	0.52	0.60	0.42
Hexanal	4.5	2.49	7.96	3.63	4.08	7.94	6.82	2.30	0.55	1.77	0.81	0.91	1.77	1.52	0.51
(<i>E</i>)-2-Hexenal	17	16.43	4.39	8.02	16.11	19.60	6.94	3.90	0.97	0.26	0.47	0.95	1.15	0.41	0.23
1-Hexanol	5.6	6.85	5.11	3.99	1.91	1.82	1.31	0.93	1.22	0.91	0.71	0.34	0.32	0.23	0.17
2-Heptanone	1	1.01	2.09	0.61	0.18	0.26	0.36	0.36	1.01	2.09	0.61	0.18	0.26	0.36	0.36
1-Octen-3-ol	1	7.36	12.51	4.60	1.93	2.31	1.96	1.28	7.36	12.51	4.60	1.93	2.31	1.96	1.28
α -Phellandrene	36	88.11	130.62	73.10	36.42	38.41	30.78	28.00	2.45	3.63	2.03	1.01	1.07	0.86	0.78
β -Myrcene	15	88.16	130.90	73.13	36.41	38.48	30.78	28.02	5.88	8.73	4.88	2.43	2.57	2.05	1.87
<i>o</i> -Cymene	11.4	14.66	16.27	7.63	3.21	3.15	2.62	1.94	1.29	1.43	0.67	0.28	0.28	0.23	0.17
β -Ocimene	0.02	29.72	40.40	24.50	11.58	12.72	9.62	9.10	1485.87	2020.19	1225.20	578.85	635.82	480.95	455.01
3,5-Octadien-2-one	0.5	13.30	21.30	14.64	6.67	11.32	5.22	1.81	26.59	42.60	29.28	13.35	22.64	10.44	3.63
Linalool	0.22	141.23	210.87	109.38	47.01	45.98	37.29	31.93	641.97	958.49	497.16	213.70	209.02	169.52	145.13
Decanal	5	13.37	8.49	6.08	0.33	0.20	0.21	4.07	2.67	1.70	1.22	0.07	0.04	0.04	0.81
Methyl salicylate	40	126.18	218.76	220.82	93.92	119.58	61.99	53.49	3.15	5.47	5.52	2.35	2.99	1.55	1.34
β -Cyclocitral	3	69.21	121.19	125.74	52.26	67.02	33.52	28.75	23.07	40.40	41.91	17.42	22.34	11.17	9.58

β -Citral	53	383.03	607.54	427.69	257.35	291.93	232.73	186.95	7.23	11.46	8.07	4.86	5.51	4.39	3.53
Citral	30	282.82	685.14	26.26	17.29	19.82	106.03	66.47	9.43	22.84	0.88	0.58	0.66	3.53	2.22
β -Ionone	0.01	8.95	17.60	11.37	6.31	7.80	4.10	3.80	895.11	1759.80	1136.86	631.48	780.28	409.87	379.56

rOAVs represents the relative odor activity values of volatile compounds.

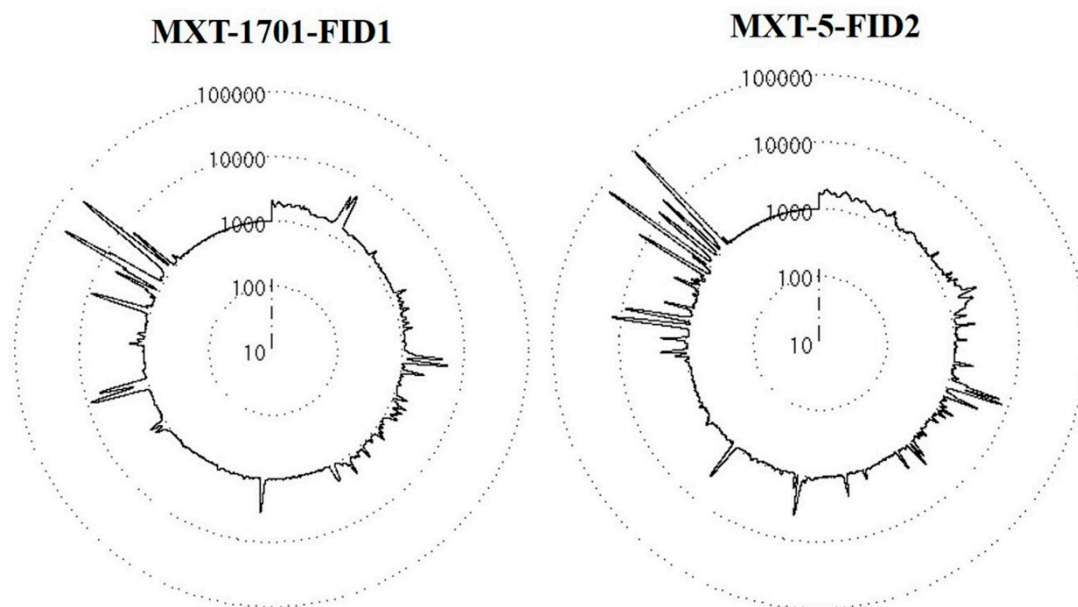


Fig. S1 Radar map of sweet and floral aroma black tea in final firing stage by using GC-E-Nose.

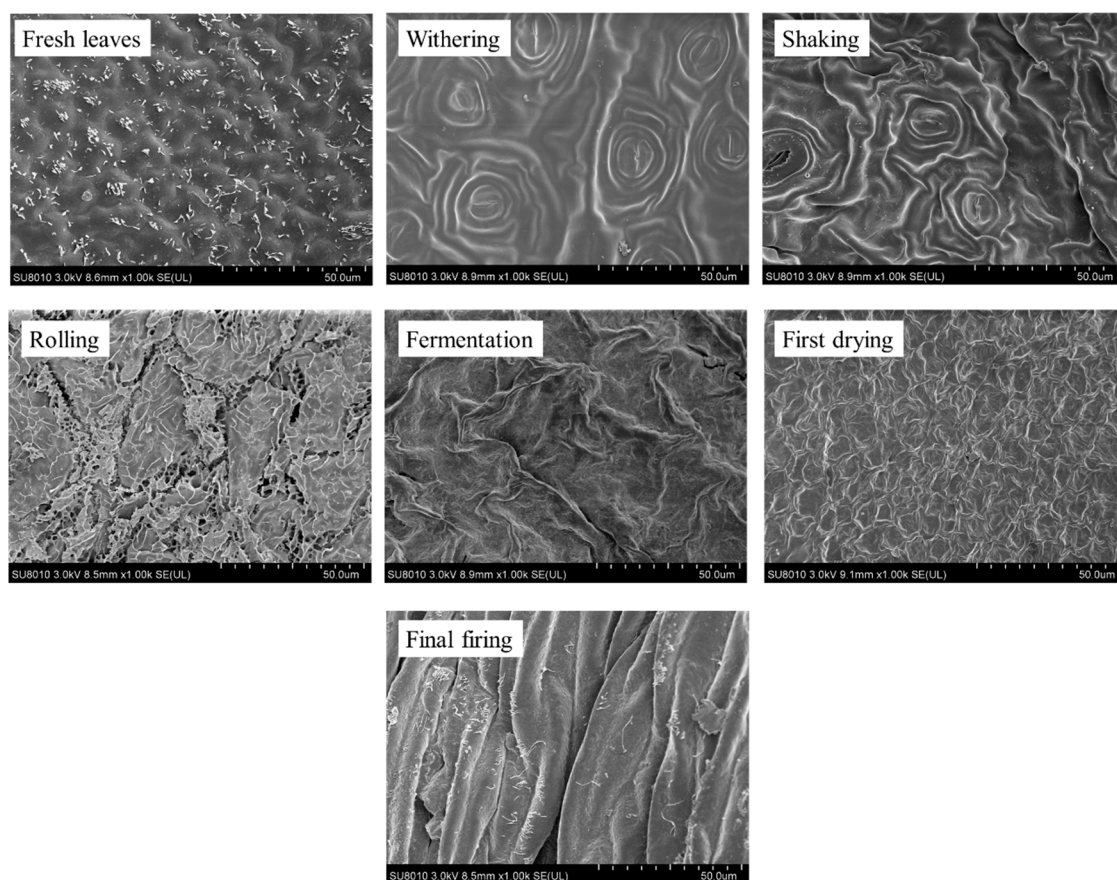


Fig. S2 The microstructures of sweet and floral aroma black tea during the manufacturing process obtained from scanning electron microscopy.