

Table S1. Roasting conditions for preparing the Wuyi rock tea samples

Tea sample	Roasting temperature (°C)	Roasting duration (h)
SX-L	120-125	5.0-5.5
SX- M	130-135	10.0-10.5
SX-S	130-135	14.0-15.0
QZ- L	120-125	5.0-5.5
QZ- M	130-135	10.0-10.5
QZ- S	130-135	14.0-15.0
DHP- L	120-125	5-5.5
DHP- M	130-135	10.0-10.5
DHP- S	130-135	14.0-15.0
RG- L	120-125	5-5.5
RG- M	130-135	10.0-10.5
RG- S	130-135	14.0-15.0

L, M and S represent low, moderate and sufficient roasting degree, respectively. Samples may be in little different conditions before roasting, which is not easy to control when processing, so the temperature and time may be slightly changed to make it similar with the real practical production.

Table S2. Category and relative content (%) of volatile compounds

Tea samples	Compound number (relative content, %)											Total
	Alcohols	Esters	Nitrogen heterocyclic compounds	Oxygen heterocyclic compounds	Aromatic hydrocarbons	Ketones	Aldehydes	Alkanes	Olefins	Acids	Sulphur compounds	
SX-L	15 (23.66)	12 (12.98)	11 (7.42)	9 (10.34)	7 (8.79)	6 (11.94)	6 (5.95)	6 (6.62)	3 (8.91)	1 (0.53)	2 (2.83)	78
SX-M	13 (24.61)	12 (9.90)	7 (19.40)	4 (3.99)	7 (16.84)	5 (4.43)	1 (8.58)	4 (4.84)	5 (5.44)	1 (1.44)	2 (0.54)	61
SX-S	14 (21.52)	15 (14.32)	11 (16.04)	7 (5.39)	6 (11.70)	7 (6.68)	4 (7.51)	5 (6.40)	10 (6.63)	4 (1.05)	2 (2.77)	85
QZ-L	22 (31.20)	15 (17.99)	15 (17.83)	11 (5.72)	5 (4.15)	5 (7.59)	2 (1.80)	4 (4.37)	4 (5.05)	2 (1.21)	2 (3.08)	87
QZ-M	27 (32.47)	13 (21.79)	10 (10.94)	9 (6.70)	5 (8.57)	5 (3.74)	3 (3.01)	3 (4.02)	6 (7.01)	1 (0.25)	2 (1.50)	84
QZ-S	23 (35.74)	8 (14.29)	12 (14.59)	6 (2.83)	6 (10.46)	6 (4.14)	3 (3.76)	5 (6.38)	4 (2.41)	3 (3.20)	2 (2.20)	78
DHP-L	24 (31.38)	12 (19.38)	8 (9.33)	10 (10.54)	6 (6.47)	6 (3.73)	3 (4.21)	3 (2.76)	6 (9.24)	2 (1.35)	2 (1.62)	82
DHP-M	23 (27.87)	11 (16.98)	9 (13.21)	7 (8.03)	6 (8.34)	5 (1.91)	5 (9.59)	4 (4.87)	6 (6.39)	2 (1.04)	3 (1.77)	81
DHP-S	18 (19.86)	13 (15.23)	11 (13.20)	8 (12.45)	6 (9.44)	5 (2.66)	6 (16.50)	4 (3.97)	5 (3.08)	2 (2.16)	2 (1.44)	80
RG-L	6 (24.47)	6 (5.62)	13 (9.81)	13 (9.38)	10 (8.79)	9 (11.47)	3 (1.71)	18 (21.34)	6 (6.28)	1 (0.65)	1 (0.48)	86
RG-M	19 (27.34)	15 (13.88)	8 (11.00)	7 (6.02)	6 (10.40)	6 (2.17)	1 (0.81)	4 (4.65)	8 (22.91)	1 (0.19)	2 (0.63)	77
RG-S	21 (27.37)	14 (28.26)	11 (12.40)	7 (2.96)	9 (9.06)	6 (3.07)	0 (0)	3 (3.46)	8 (11.85)	1 (0.22)	2 (1.35)	82

Table S3. Volatile compounds and their relative contents in 12 Wuyi rock tea samples

Volatile compounds	N	Relative content (%)			
		Min	Max	Mean	SD
Hexanoic acid, 3-hexenyl ester, (Z)-	12	0.63	3.57	2.11	0.86
Hexanoic acid, hexyl ester	12	0.72	3.25	1.81	0.76
3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	12	0.40	6.37	1.66	1.64
Hexanoic acid, 2-hexenyl ester, (E)-	12	0.33	1.41	0.78	0.33
1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-	11	2.11	19.14	7.66	4.97
Hydrazinecarboxylic acid, phenylmethyl ester	11	0.66	6.67	3.10	1.84
Tetradecane, 2,6,10-trimethyl-	11	1.50	4.49	2.58	0.97
Formic acid, 3,7,11-trimethyl-1,6,10-dodecatrien-3-yl ester	11	0.28	5.91	2.57	1.85
7-Methyl-Z-tetradecen-1-ol acetate	11	0.35	4.91	2.17	1.35
Limonen-6-ol, pivalate	11	0.54	4.38	1.76	1.04
2-Octen-1-ol, 3,7-dimethyl-, isobutyrate, (Z)-	11	0.23	4.02	1.58	1.32
Geranyl isovalerate	11	0.61	3.47	1.57	0.97
1,6-Octadien-3-ol, 3,7-dimethyl-	11	0.76	1.58	1.04	0.28
4-(2,4,4-Trimethyl-cyclohexa-1,5-dienyl)-but-3-en-2-one	11	0.14	2.77	0.95	0.95
1-Heptatriacotanol	11	0.09	2.74	0.92	0.84
tert-Hexadecanethiol	11	0.12	1.64	0.87	0.48
Disulfide, di-tert-dodecyl	11	0.27	1.94	0.86	0.58
.alpha.-Farnesene	10	1.12	6.27	3.28	1.83
.alpha.-Methyl-.alpha.-[4-methyl-3-pentenyl]oxiranemethanol	10	0.33	3.97	2.24	1.19
1,2-15,16-Diepoxyhexadecane	10	0.23	4.74	2.21	1.49
D-Limonene	10	0.52	3.17	1.19	0.78
Phytol, acetate	10	0.15	4.36	1.09	1.24
Octadecane, 1-chloro-	10	0.25	1.61	0.86	0.38
3-Isopropylidene-5-methyl-hex-4-en-2-one	10	0.23	1.67	0.80	0.43
3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	10	0.17	1.53	0.53	0.41
Dodecane, 2-methyl-	10	0.26	0.45	0.36	0.06
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(2-methyloxiranyl)-	9	0.25	2.14	1.11	0.76
2,5-Octadecadiynoic acid, methyl ester	9	0.32	2.33	0.88	0.64
Naphthalene, 1,2,3,4-tetrahydro-1,6,8-trimethyl-	9	0.12	1.13	0.77	0.28
p-Xylene	8	1.16	6.02	3.91	1.62
2,5-Dimethylcyclohexanol	8	2.37	4.33	2.99	0.68
1, 1, 5-Trimethyl-1, 2-dihydronaphthalene	8	0.42	3.07	2.22	0.88
2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	8	0.71	4.09	1.62	1.18
6-Benzyloxy-2,6-dimethyl-octa-2,7-dien-1-ol	8	0.11	1.53	0.71	0.54
4-(2,5-Dihydro-3-methoxyphenyl)butylamine	8	0.19	1.26	0.71	0.38
.alpha.-acorenol	8	0.18	1.43	0.57	0.40
Butanoic acid, 2-methyl-, hexyl ester	8	0.23	0.90	0.55	0.27
Phenol, 4-(ethylamino)-	8	0.18	1.05	0.43	0.29
Acetic acid, (1,2,3,4,5,6,7,8-octahydro-3,8,8-trimethylnaphth-2-yl)methyl ester	8	0.21	0.72	0.42	0.20

Acetamide, N-(4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-yl)-, (1.alpha.,2.beta.,5.alpha.)-	8	0.11	0.61	0.41	0.20
4-epi-cubedol	8	0.08	0.18	0.13	0.04
(2,2,6-Trimethyl-bicyclo[4.1.0]hept-1-yl)-methanol	7	0.32	3.30	1.44	0.92
Cyclopentanone, 2-cyclopentylidene-	7	0.17	1.18	0.58	0.44
1-Methoxyadamantane	7	0.37	0.76	0.57	0.13
Undec-10-ynoic acid	7	0.22	0.57	0.37	0.15
O-Methylisourea	6	0.94	5.38	2.90	1.72
Isopilocarpine	6	0.71	2.43	1.69	0.57
Hexanal	6	0.38	2.38	1.46	0.82
Nerolidyl acetate	6	0.19	2.52	1.12	0.92
5-Ethyl-5-methyl-2-phenyl-2-oxazoline	6	0.30	2.57	0.99	0.86
2,6-Octadiene-1,8-diol, 2,6-dimethyl-	6	0.11	2.34	0.88	0.78
1,1-Cyclohexanedimethanol	6	0.08	2.16	0.72	0.74
E-10-Methyl-11-tetradecen-1-ol propionate	6	0.25	1.13	0.66	0.37
2-Methyl-4-(2,6,6-trimethylcyclohex-2-enyl)but-3-en-2-ol	6	0.34	0.55	0.45	0.07
3,7-Octadiene-2,6-diol, 2,6-dimethyl-	6	0.27	0.65	0.41	0.15
2-Butyloxycarbonyloxy-1,1,10-trimethyl-6,9-epidioxydecalin	6	0.11	0.53	0.36	0.19
3-Cyclohexen-1-carboxaldehyde, 3,4-dimethyl-	5	2.75	8.14	4.63	2.23
Pentadecane	5	0.94	5.50	2.18	1.89
Cyclohexanol, 4-methyl-, trans-	5	1.04	3.05	1.99	0.86
Terpinyl formate	5	1.35	2.81	1.94	0.61
Benzenepropanoic acid, .alpha.-(hydroxyimino)-	5	1.04	3.18	1.77	0.86
cis-.beta.-Farnesene	5	0.58	2.15	1.39	0.68
10-Heptadecen-8-ynoic acid, methyl ester, (E)-	5	0.55	0.98	0.86	0.19
Heptadecane, 2,6,10,15-tetramethyl-	5	0.38	1.47	0.85	0.40
10-Undecynoic acid, methyl ester	5	0.26	1.43	0.74	0.49
Z,Z-2,5-Pentadecadien-1-ol	5	0.31	1.05	0.57	0.29
Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	5	0.21	0.58	0.35	0.15
7-epi-cis-sesquisabinene hydrate	5	0.09	0.43	0.27	0.16
Octahydrobenzo[b]pyran, 4a-acetoxy-5,5,8a-trimethyl-	5	0.12	0.35	0.20	0.10
[5,5-Dimethyl-6-(3-methyl-buta-1,3-dienyl)-7-oxa-bicyclo[4.1.0]hept-1-yl]-methanol	5	0.09	0.28	0.18	0.08
Octadecanal, 2-bromo-	5	0.06	0.18	0.13	0.05
2,4-Heptadienal, (E,E)-	4	0.86	5.65	2.23	2.29
Tricyclo[2.2.1.0(2,6)]heptan-3-ol, 4,5,5-trimethyl-	4	0.44	3.32	1.96	1.44
Benzaldehyde	4	0.22	3.99	1.95	1.55
Tricyclo[4.2.2.0(1,5)]decan-7-ol	4	1.16	1.54	1.38	0.17
Fumaric acid, 2-methylcyclohex-1-enylmethyl pentadecyl ester	4	0.67	1.83	1.30	0.53
3-Decanynoic acid	4	0.58	1.60	1.03	0.42
E-2-Hexenyl benzoate	4	0.43	1.43	1.02	0.48
Benzaldehyde, 3-benzyloxy-2-fluoro-4-methoxy-	4	0.12	2.81	0.95	1.25
1,5,5-Trimethyl-6-methylene-cyclohexene	4	0.11	2.01	0.89	0.83

cis-3-Hexenyl-.alpha.-methylbutyrate	4	0.53	0.88	0.73	0.17
Ethinamate	4	0.16	1.42	0.72	0.64
N-[3-[N-Aziridyl]propylidene]tetrahydrofurfurylamine	4	0.51	0.90	0.70	0.18
2-Ethylbutyric acid, eicosyl ester	4	0.40	0.73	0.58	0.15
Z,Z,Z-1,4,6,9-Nonadecatetraene	4	0.51	0.63	0.57	0.06
Piperazine, 1-methyl-4-[2-(p-tolylsulfonyl)ethyl]-	4	0.22	0.66	0.45	0.21
trans-Farnesol	4	0.20	0.41	0.33	0.09
2-Pentadecanone, 6,10,14-trimethyl-	4	0.12	0.30	0.23	0.08
2,4-Nonadienal, (E,E)-	3	2.24	5.35	3.28	1.79
Cyclohexan-1,4,5-triol-3-one-1-carboxylic acid	3	0.59	5.59	2.31	2.85
2,2,2-Trifluoro-N-[2-(1-hydroxy-2,2,6,6-tetramethyl-piperidin-4-yl)-ethyl]-acetamide	3	0.13	3.99	1.86	1.96
Mesitylene	3	1.16	2.07	1.56	0.46
Heptane, 1-nitro-	3	1.04	1.81	1.52	0.42
1,2-Propanediol diformate	3	0.82	1.40	1.20	0.33
2H-Pyran-3-ol, 6-ethenyltetrahydro-2,2,6-trimethyl-	3	0.61	1.46	1.15	0.47
Bicyclo[3.1.1]hept-2-en-4-ol, 2,6,6-trimethyl-, acetate	3	0.61	1.37	1.10	0.43
Cyclohexene, 1-(2-nitro-2-propenyl)-	3	0.58	1.40	1.04	0.42
1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl-	3	0.61	1.42	1.01	0.41
5-Amino-1-benzoyl-1H-pyrazole-3,4-dicarbonitrile	3	0.24	1.18	0.86	0.54
Imidazole, 4-methyl-5-[2-methyl-2-propenyl]-	3	0.57	1.08	0.79	0.26
Naphthalene, 1,2,3,4-tetrahydro-1,5,8-trimethyl-	3	0.65	0.87	0.78	0.11
R-Limonene	3	0.20	1.13	0.61	0.47
(9-Oxabicyclo[3.3.1]non-6-en-3-yl)methanol	3	0.40	0.74	0.58	0.17
Nona-3,5-dien-2-ol	3	0.43	0.81	0.57	0.20
Cyclopentasiloxane, decamethyl-	3	0.48	0.62	0.55	0.07
3,7-Cycloundecadien-1-ol, 1,5,5,8-tetramethyl-	3	0.41	0.56	0.47	0.07
17-Octadecynoic acid	3	0.08	0.93	0.47	0.43
(-)-Myrtenol	3	0.32	0.57	0.42	0.13
Ethanone, 1-(1-hydroxy-2,6,6-trimethyl-2,4-cyclohexadien-1-yl)-	3	0.40	0.44	0.42	0.02
1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]-	3	0.35	0.51	0.42	0.08
Heptacosane	3	0.10	0.72	0.31	0.35
5-Hydroxymethyl-1,1,4a-trimethyl-6-methylenedecahydronaphthalen-2-ol	3	0.09	0.48	0.29	0.20
10-Hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,12b,13,14b-eicosahydricene-2-carboxylic acid	3	0.10	0.35	0.24	0.13
N-Benzyl-2-aminocinnamate, methyl ester	3	0.16	0.23	0.20	0.03
Oct-3-ene-1,5-diyne, 3-t-butyl-7,7-dimethyl-	3	0.12	0.25	0.19	0.06
Cedrol	3	0.14	0.24	0.18	0.05
Phenol, 2,4,6-tris(1,1-dimethylethyl)-	3	0.12	0.14	0.13	0.01
3-Buten-2-ol, 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	3	0.10	0.13	0.11	0.02
Bromoacetic acid, 2-ethylcyclohexyl ester	2	2.24	5.01	3.63	1.96

2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-	2	2.16	4.02	3.09	1.32
2-Oxabicyclo[2.2.2]octan-6-ol, 1,3,3-trimethyl-, acetate	2	2.01	4.10	3.05	1.47
2,2-Difluoroethanol, tert-butyldimethylsilyl ether	2	2.44	3.00	2.72	0.40
2,7-Octadiene-1,6-diol, 2,6-dimethyl-	2	2.27	3.05	2.66	0.56
3-Carene	2	1.56	2.90	2.23	0.95
Phenol, 4-amino-3-methyl-	2	1.22	2.83	2.02	1.14
Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	2	1.58	1.59	1.59	0.00
1H-Pyrrole, 2-ethyl-	2	1.45	1.60	1.52	0.10
1-(4-tert-Butylphenyl)propan-2-one	2	1.45	1.53	1.49	0.06
Naphthalene, 1,2-dihydro-1,5,8-trimethyl-	2	1.00	1.78	1.39	0.55
Acetic acid, 1,3,7-trimethylocta-2,6-dienyl ester	2	0.94	1.48	1.21	0.38
Pyrazine, 2-ethyl-3,5-dimethyl-	2	0.99	1.38	1.18	0.27
Caryophyllene	2	1.12	1.16	1.14	0.03
7-Propylidene-bicyclo[4.1.0]heptane	2	0.84	1.34	1.09	0.36
8-Decen-2-one, 9-methyl-5-methylene-	2	0.62	1.19	0.90	0.40
2H-Pyran-2,5-diol, tetrahydro-, diacetate	2	0.72	0.95	0.84	0.17
Cyclohexanone, 2,2,6-trimethyl-	2	0.46	1.01	0.74	0.39
3-(1,5-Dimethyl-hex-4-enyl)-2,2-dimethyl-cyclopent-3-enol	2	0.49	0.85	0.67	0.26
2,5-Pyrrolidinedione, 1-ethyl-	2	0.37	0.53	0.45	0.11
1-Penten-3-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	2	0.36	0.51	0.44	0.11
Carveol	2	0.40	0.45	0.43	0.04
Acetic acid, 10,11-dihydroxy-3,7,11-trimethyl-dodeca-2,6-dienyl ester	2	0.30	0.34	0.32	0.03
2,4-Heptadienal, 2,4-dimethyl-	2	0.20	0.38	0.29	0.13
(3-Fluorophenyl) methanol, 3-methylbutyl ether	2	0.24	0.32	0.28	0.06
Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene-	2	0.15	0.36	0.25	0.15
Ethyl iso-allocholate	2	0.24	0.26	0.25	0.02
1H-3a,7-Methanoazulene, octahydro-3,8,8-trimethyl-6-methylene-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]-	2	0.18	0.30	0.24	0.08
Hexadecanoic acid, methyl ester	2	0.19	0.29	0.24	0.07
2,4-Di-t-butyladamantane-2,4-diol	2	0.21	0.24	0.23	0.02
1b,4a-Epoxy-2H-cyclopenta[3,4]cyclopropa[8,9]cycloundec[1,2-b]oxiren-5(1aH)-one, 2,7,9,10-tetrakis(acetyloxy)decahydro-3,6,8,8,10a-pentamethyl-	2	0.09	0.32	0.21	0.17
Pentadecanoic acid, 13-methyl-, methyl ester	2	0.17	0.20	0.19	0.02
Butanoic acid, 3-methyl-, 2-hexenyl ester, (E)-	2	0.12	0.20	0.16	0.06
Bicyclo[3.1.0]hexan-2-ol, acetate, (1.alpha.,2.beta.,5.alpha.)-	2	0.11	0.19	0.15	0.06
6-epi-shyobunol	2	0.14	0.14	0.14	0.00
Propanoic acid, 2-(3-acetoxy-4,4,14-trimethylandro-8-en-17-yl)-	2	0.10	0.17	0.14	0.05
Cedrane, 8-propoxy-	2	0.11	0.12	0.12	0.00
E-2-Methyl-3-tetradecen-1-ol acetate	2	0.07	0.15	0.11	0.05
Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	2	0.09	0.12	0.11	0.02
Tetrapentacontane, 1,54-dibromo-	2	0.10	0.11	0.10	0.00

10-Methyl-8-tetradecen-1-ol acetate	2	0.06	0.13	0.09	0.05
o-Xylene	1	9.86	9.86	9.86	/
1-Bromo-3,7-dimethyl-2,6-octadiene	1	6.64	6.64	6.64	/
1,3-Hexadiene, 3-ethyl-2-methyl-, (Z)-	1	4.95	4.95	4.95	/
Hexadecane, 2,6,11,15-tetramethyl-	1	3.16	3.16	3.16	/
6-(3,5-Dimethyl-1H-pyrazol-1-yl)-N-benzyl-1,2,4,5-tetrazine-3-amine	1	3.01	3.01	3.01	/
cis-Verbenol	1	2.79	2.79	2.79	/
Benzyl nitrile	1	2.68	2.68	2.68	/
trans-.beta.-Ionone	1	2.67	2.67	2.67	/
Tributyl phosphate	1	2.63	2.63	2.63	/
trans-8-Isopropylbicyclo[4.3.0]non-3-ene	1	2.41	2.41	2.41	/
1,2-Dihydrothujopsene-(I1)	1	2.21	2.21	2.21	/
4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one	1	2.19	2.19	2.19	/
1,5,7-Octatrien-3-ol, 3,7-dimethyl-	1	2.16	2.16	2.16	/
Octanoic acid, 3-phenyl-2-propenyl ester	1	2.06	2.06	2.06	/
Benzene, [[[1-ethenyl-1,5-dimethyl-4-hexenyl)oxy]methyl]-	1	2.05	2.05	2.05	/
Oxirane, decyl-	1	2.03	2.03	2.03	/
Hexadecane	1	2.01	2.01	2.01	/
Linalyl acetate	1	2.00	2.00	2.00	/
1,4-Benzenediamine	1	1.96	1.96	1.96	/
Ethyl 2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate	1	1.88	1.88	1.88	/
2,6,10-Trimethyltridecane	1	1.85	1.85	1.85	/
Decanoic acid, ethyl ester	1	1.83	1.83	1.83	/
N-Methoxy-1-ribofuranosyl-4-imidazolecarboxylic amide	1	1.79	1.79	1.79	/
Benzene, 1,2-diethyl-	1	1.78	1.78	1.78	/
Bicyclo[2.2.1]heptane, 7,7-dimethyl-2-methylene-	1	1.77	1.77	1.77	/
2-Hydroxy-2-(5-methylfuran-2-yl)1-phenylethanone	1	1.75	1.75	1.75	/
Tetraacetyl-d-xylonic nitrile	1	1.73	1.73	1.73	/
1,5,9-Cyclododecanetriol	1	1.67	1.67	1.67	/
Nonane, 3-methyl-5-propyl-	1	1.54	1.54	1.54	/
Geranyl vinyl ether	1	1.49	1.49	1.49	/
Menthol, 1'-(butyn-3-one-1-yl)-, (1R,2S,5R)-	1	1.44	1.44	1.44	/
2-Isopropyl-5-methyl-1-heptanol	1	1.42	1.42	1.42	/
Cyclohexanol, 2-methyl-5-(1-methylethenyl)-	1	1.36	1.36	1.36	/
4-Amino-2,3-xyleneol	1	1.32	1.32	1.32	/
Nonyl tetradecyl ether	1	1.22	1.22	1.22	/
Pentadioic acid, dihydrazide, N2,N2'-bis(2-furfurylideno)-	1	1.21	1.21	1.21	/
(3R,6S)-2,2,6-Trimethyl-6-vinyltetrahydro-2H-pyran-3-ol	1	1.19	1.19	1.19	/
2-Nonen-1-ol	1	1.16	1.16	1.16	/
1H-Benzocyclohepten-7-ol, 2,3,4,4a,5,6,7,8-octahydro-1,1,4a,7-tetramethyl-, cis-	1	1.15	1.15	1.15	/
5-Hepten-2-one, 6-methyl-	1	1.07	1.07	1.07	/
sec-Butyl nitrite	1	1.00	1.00	1.00	/
Linalool	1	0.99	0.99	0.99	/

(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	1	0.99	0.99	0.99	/
1-Propanone, 1-(1-adamantyl)-3-dimethylamino-	1	0.94	0.94	0.94	/
Toluene	1	0.93	0.93	0.93	/
2-Decen-1-ol, (E)-	1	0.92	0.92	0.92	/
.alpha.-Ionone	1	0.91	0.91	0.91	/
.gamma.-Chlorobutyrophenone	1	0.90	0.90	0.90	/
2-Benzoyloxy-1,1,10-trimethyl-6,9-epidioxydecalin	1	0.89	0.89	0.89	/
10-Methyl-E-11-tridecen-1-ol propionate	1	0.89	0.89	0.89	/
Ethanone, 1-(1H-pyrrol-2-yl)-	1	0.87	0.87	0.87	/
3-(O-Anisidinomethyl)-5-(3-fluorobenzylidene)-2,4-thiazolidinedione	1	0.85	0.85	0.85	/
Bicyclo[4.1.0]hepta-1,3,5-triene	1	0.85	0.85	0.85	/
Imidazo[4,5-d]imidazole, 1,6-dihydro-	1	0.78	0.78	0.78	/
3-Formyl-4,5-dimethyl-pyrrole	1	0.76	0.76	0.76	/
Spiro[2,4]hepta-4,6-diene	1	0.76	0.76	0.76	/
Benzenemethanol, 3-amino-	1	0.76	0.76	0.76	/
3,5-Heptadienal, 2-ethylidene-6-methyl-	1	0.75	0.75	0.75	/
3-Furaldehyde	1	0.73	0.73	0.73	/
2-Hepten-1-ol, (E)-	1	0.72	0.72	0.72	/
Pyrazine, 2-ethyl-6-methyl-	1	0.69	0.69	0.69	/
Nonane, 4,5-dimethyl-	1	0.69	0.69	0.69	/
Furan, 2-propyl-	1	0.68	0.68	0.68	/
3-Pentanone	1	0.68	0.68	0.68	/
Heptadecane, 2-methyl-	1	0.67	0.67	0.67	/
5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	1	0.66	0.66	0.66	/
1-Propanone, 1-(2-furanyl)-	1	0.65	0.65	0.65	/
Propanoic acid, anhydride	1	0.65	0.65	0.65	/
Neophytadiene	1	0.65	0.65	0.65	/
1-(4-Methoxyphenyl)propane-1,2-diol	1	0.64	0.64	0.64	/
5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	1	0.63	0.63	0.63	/
Nonane, 5-butyl-	1	0.61	0.61	0.61	/
Nonane, 2,2,4,4,6,8,8-heptamethyl-	1	0.57	0.57	0.57	/
2H-Pyran, tetrahydro-2-(12-pentadecyloxy)-	1	0.55	0.55	0.55	/
11-Methyldodecanol	1	0.55	0.55	0.55	/
Methoxyacetic acid, pentyl ester	1	0.54	0.54	0.54	/
1,7-Octadien-3-ol, 3,7-dimethyl-	1	0.53	0.53	0.53	/
1-Decanol, 2-hexyl-	1	0.52	0.52	0.52	/
2-Furancarboxaldehyde, 5-methyl-	1	0.52	0.52	0.52	/
3-Acetyl-N-methyl-tomatidine	1	0.52	0.52	0.52	/
Furan, 2-ethyl-5-methyl-	1	0.51	0.51	0.51	/
2-Adamantanol, 4-bromo-	1	0.51	0.51	0.51	/
2H-Benzo[f]oxireno[2,3-E]benzofuran-8(9H)-one, 9-[[[2-(dimethylamino)ethyl]amino]methyl]octahydro-2,5a-dimethyl-	1	0.51	0.51	0.51	/
Pyrazine, trimethyl-	1	0.50	0.50	0.50	/
1-Hexadecanol, 2-methyl-	1	0.50	0.50	0.50	/

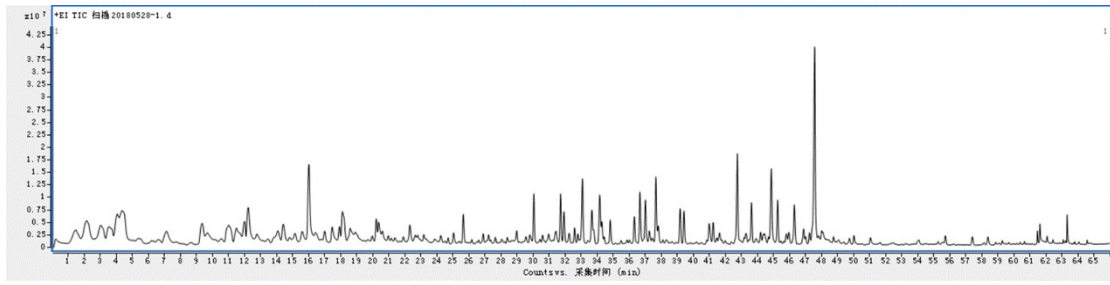
Decane-1-sulfonic acid (4-methoxy-phenyl)-amide	1	0.48	0.48	0.48	/
8-Tetradecyn-1-ol acetate	1	0.48	0.48	0.48	/
3-Benzoyl-perhydro-2-oxofuran	1	0.47	0.47	0.47	/
Undecane, 3,8-dimethyl-	1	0.45	0.45	0.45	/
p-Cymene	1	0.45	0.45	0.45	/
1H-Imidazole-4-ethanamine, .beta.-methyl-	1	0.45	0.45	0.45	/
Pentanoic acid, heptadecyl ester	1	0.45	0.45	0.45	/
2,4,6-Trimethyl-1,3-phenylenediamine	1	0.45	0.45	0.45	/
2,4-Difluorobenzene, 1-benzyloxy-	1	0.44	0.44	0.44	/
1-Pentyne, 3-ethoxy-3-ethyl-	1	0.43	0.43	0.43	/
2-Bromo dodecane	1	0.43	0.43	0.43	/
trans-Linalool oxide (furanoid)	1	0.42	0.42	0.42	/
6-Amino-2,4-dimethylphenol	1	0.41	0.41	0.41	/
E-6-Tetradecen-1-ol acetate	1	0.41	0.41	0.41	/
2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-, cis-	1	0.40	0.40	0.40	/
Cyclohexene, 3-(1-methylethyl)-	1	0.40	0.40	0.40	/
Tricyclo[5.3.0.0(2,6)]deca-3,10-dione, 6,7-dichloro-	1	0.40	0.40	0.40	/
Heneicosane	1	0.40	0.40	0.40	/
4-Acetyl-1H-pyrroline-2-carbaldehyde	1	0.39	0.39	0.39	/
Hexadecane, 2,6,10,14-tetramethyl-	1	0.39	0.39	0.39	/
1-Octanesulfonyl chloride	1	0.39	0.39	0.39	/
1,3,7-Octatriene, 2,7-dimethyl-	1	0.39	0.39	0.39	/
6,6-Dimethyl-10-methylene-1-oxa-spiro[4.5]decane	1	0.38	0.38	0.38	/
2-Pentadecen-4-yne, (Z)-	1	0.38	0.38	0.38	/
Benzeneacetaldehyde	1	0.38	0.38	0.38	/
6-Methyl-6-nitroheptan-2-one	1	0.37	0.37	0.37	/
Geranyl angelate	1	0.37	0.37	0.37	/
2-Propanone, 1,1,1-trifluoro-	1	0.37	0.37	0.37	/
3,5-Dimethyl-4-allylpyrazole	1	0.37	0.37	0.37	/
Ethanone, 1-(2-furanyl)-	1	0.36	0.36	0.36	/
Pyrazine, 2-ethyl-3-methyl-	1	0.36	0.36	0.36	/
(-)-Spathulenol	1	0.34	0.34	0.34	/
Octanoic acid, 7-oxo-	1	0.33	0.33	0.33	/
1,2-Cyclopentanediol, 3-methyl-	1	0.33	0.33	0.33	/
3-Ethyl-3-methylheptane	1	0.32	0.32	0.32	/
Tetradecane	1	0.31	0.31	0.31	/
3-t-Butyl-oct-6-en-1-ol	1	0.31	0.31	0.31	/
1-Cyclopropene-1-pentanol, .alpha.,.epsilon.,.epsilon.,2-tetramethyl- 3-(1-methylethenyl)-	1	0.30	0.30	0.30	/
1,8-Nonadien-3-ol	1	0.30	0.30	0.30	/
1,4-dihydroxy-p-menth-2-ene	1	0.27	0.27	0.27	/
Phenol, 2,4,6-tri-tert-butyl-	1	0.27	0.27	0.27	/
2,4-Dimethyldodecane	1	0.27	0.27	0.27	/

Bicyclo[2.2.1]heptan-2-ol, 7,7-dimethyl-, acetate	1	0.26	0.26	0.26	/
5-Hexadecenoic acid, 2-methoxy-, methyl ester	1	0.26	0.26	0.26	/
Octanal	1	0.24	0.24	0.24	/
Pyrazine, 3-ethyl-2,5-dimethyl-	1	0.24	0.24	0.24	/
4-(2,2-Dimethyl-6-methylenecyclohexyl)butanal	1	0.21	0.21	0.21	/
3-Methoxymethoxy-6,6-dimethyl-2-methylene-bicyclo[3.1.1]heptane	1	0.21	0.21	0.21	/
1H-3a,7-Methanoazulene, 2,3,6,7,8,8a-hexahydro-1,4,9,9-tetramethyl-, (1.alpha.,3a.alpha.,7.alpha.,8a.beta.)-	1	0.20	0.20	0.20	/
Phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-	1	0.19	0.19	0.19	/
3-(Benzyloxymethyl)hex-5-ene-1,2-diol	1	0.18	0.18	0.18	/
1,4-Methanoazulen-3-ol, decahydro-1,5,5,8a-tetramethyl-, [1S-(1.alpha.,3.beta.,3a.beta.,4.alpha.,8a.beta.)]-	1	0.18	0.18	0.18	/
Octadecane, 3-ethyl-5-(2-ethylbutyl)-	1	0.17	0.17	0.17	/
2-Naphthol, 1,2,3,4,4a,5,6,7-octahydro-4a-methyl-	1	0.15	0.15	0.15	/
1,4-Methanoazulen-7-ol, decahydro-1,5,5,8a-tetramethyl-, [1S-(1.alpha.,3a.beta.,4.alpha.,7.beta.,8a.beta.)]-	1	0.14	0.14	0.14	/
Falcarinol	1	0.14	0.14	0.14	/
(1H)Imidazol-4-amine, 2,5-diisobutyl-	1	0.13	0.13	0.13	/
2-Naphthalenamine, 1,2,3,4-tetrahydro-N-methyl-1-(2-methyl-1-propenyl)-, trans-	1	0.13	0.13	0.13	/
3-Cyclopentylpropionic acid, 2-isopropoxyphenyl ester	1	0.12	0.12	0.12	/
Nona-2,3-dienoic acid, ethyl ester	1	0.12	0.12	0.12	/
2-(2-Methyl-propenyl)-cyclohexanone oxime	1	0.12	0.12	0.12	/
Acetic acid, 1,7,7-trimethyl-bicyclo[2.2.1]hept-2-yl ester	1	0.12	0.12	0.12	/
2,5,5,8a-Tetramethyl-4-methylene-6,7,8,8a-tetrahydro-4H,5H-chromen-4a-yl hydroperoxide	1	0.12	0.12	0.12	/
beta.-Guaiene	1	0.11	0.11	0.11	/
2-[4-methyl-6-(2,6,6-trimethylcyclohex-1-enyl)hexa-1,3,5-trienyl]cyclohex-1-en-1-carboxaldehyde	1	0.11	0.11	0.11	/
1,3-Dioxane, 5-(hexadecyloxy)-2-pentadecyl-, trans-	1	0.11	0.11	0.11	/
Acetamide, N-methyl-N-[4-(3-hydroxypyrrolidinyl)-2-butenyl]-	1	0.11	0.11	0.11	/
Cucurbitacin b, 25-desacetoxy-	1	0.11	0.11	0.11	/
2,4,6-Cycloheptatrien-1-one, 3,5-bis-trimethylsilyl-	1	0.09	0.09	0.09	/
Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	1	0.09	0.09	0.09	/
Oxiranedodecanoic acid, 3-octyl-, cis-	1	0.06	0.06	0.06	/

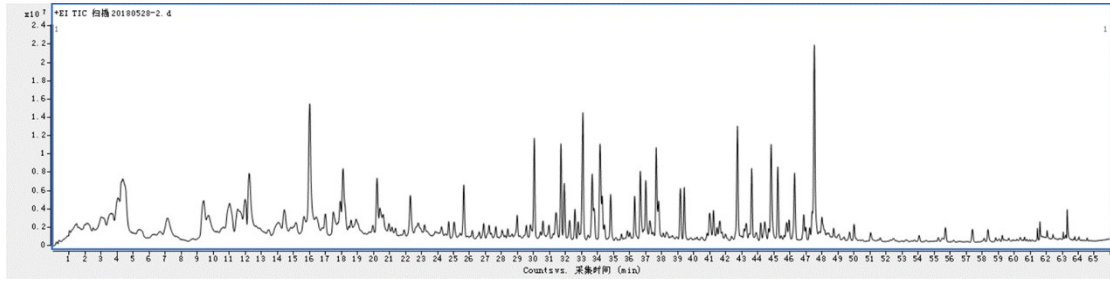
Note: the numbers are the frequency of occurrence of all the volatiles.

Fig S1. TIC of aroma for DHP samples with different roasting levels.

DHP-L



DHP-M



DHP-S

