

Supplementary Material

Table S1 VFCs in aged HBV and SV detected by HS-SPME/GC-MS

Compounds		Concentrations (mg·L ⁻¹)	
		HBV	SV
Acids	Propanoic acid, 2-methyl-	51.24±0.17	103.85±2.72
	Butanoic acid, 3-methyl-	563.83±10.40	458.56±13.12
	Butanoic acid, 2-methyl-	214.71±4.12	164.36±4.50
	Pentanoic acid, 4-methyl-	24.42±2.42	25.36±1.67
	Pentanoic acid, 3-methyl-	5.15±0.81	-
	L-Lactic acid	72.75±1.94	35.39±2.40
	Benzoic acid	56.29±0.91	98.45±2.44
	Tetradecanoic acid	19.14±0.10	33.47±2.45
	Dodecanoic acid	-	17.19±1.55
	Propanedioic acid	-	20.74±4.06
	Heptanoic acid	73.66±1.88	71.62±3.27
	Nonanoic acid	224.44±1.73	114.33±3.06
	Hexanoic acid	808.51±16.02	431.15±10.84
Alcohols	1-Butanol, 3-methyl-	58.45±2.44	10.66±0.47
	1-Butanol, 2-methyl-	28.21±2.98	5.58±0.41
	1-Pentanol	2.23±0.16	-
	2,3-Butanediol, [R-(R*,R*)]-	248.85±3.43	1043.19±30.54
	2-Furanmethanol	411.11±7.15	747.36±10.15
	1-Hexanol	2.12±0.08	-
	4,5-Octanediol, 2,7-dimethyl-	6.98±0.41	10.11±0.78
	1-Hexanol, 2-ethyl-	10.12±0.08	7.82±0.58
	Phenylethyl alcohol	1578.52±34.31	2478.52±55.52
	Cedrol	20.15±2.93	16.23±0.87
	Propylene Glycol	13.03±0.73	-
	2-Butanol, 1-methoxy-	12.08±0.76	-
	1-Propanol, 3-(methylthio)-	20.78±1.97	-
	1-Dodecanol	-	26.97±1.39
	1-Tetradecanol	-	20.21±1.56
	n-Tridecan-1-ol	20.25±1.59	20.23±0.87
	1-Decanol	-	28.31±0.93
Esters	Isobutyl acetate	3.34±0.24	-
	Propanoic acid, 2-hydroxy-, ethyl ester, (S)-	55.58±1.82	53.38±1.68
	1-Butanol, 3-methyl-, acetate	13.39±1.69	-
	1-Butanol, 2-methyl-, acetate	9.09±0.77	-
	1-Methoxy-2-propyl acetate	323.91±7.71	109.79±4.80
	2-Furanmethanol, acetate	231.23±14.30	105.97±4.22
	2,3-Butanediol, diacetate	185.17±110.02	74.59±2.54
	1,3-Propanediol, diacetate	45.37±3.80	51.41±0.99
	3-(Methylthio)propyl acetate	107.03±4.98	24.18±1.54
	Acetic acid, phenylmethyl ester	30.31±3.05	-

	Butanedioic acid, diethyl ester	148.15±2.93	109.06±1.46
	Formic acid, 2-phenylethyl ester	11.73±1.22	11.08±1.47
	Benzeneacetic acid, ethyl ester	19.33±2.35	4.06±0.75
	Acetic acid, 2-phenylethyl ester	1193.05±32.56	495.92±7.01
	l-(+)-Ascorbic acid 2,6-dihexadecanoate	55.17±1.53	112.59±3.95
	Dibutyl phthalate	207.09±6.43	210.07±7.12
	Hexadecanoic acid, ethyl ester	34.51±2.48	58.77±2.67
	Ethyl Acetate	10.12±1.50	16.15±1.52
	n-Caproic acid vinyl ester	19.06±1.46	48.12±2.83
	Allyl 2-ethyl butyrate	10.04±0.74	-
	Phenol, 4-methoxy-, acetate	40.13±2.21	-
	n-Propyl acetate	0.82±0.16	-
	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	-	7.12±0.79
	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	-	49.37±2.38
	Benzoic acid, 4-hydroxy-3-methoxy-, ethyl ester	-	7.09±0.77
	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1.alpha.,2.alpha.,5.alpha.)-	-	3.75±0.32
	Butyrolactone	-	1.02±0.27
Aldehydes	Hexanal	14.62±0.44	28.81±2.69
	3-Furaldehyde	95.88±2.74	367.65±4.70
	Methional	3.12±0.79	20.21±2.27
	Benzaldehyde	414.71±3.33	303.41±2.41
	Benzeneacetaldehyde	114.65±3.29	203.71±2.62
	Nonanal	43.57±1.82	55.71±2.63
	Decanal	37.76±1.24	38.67±2.59
	2-Phenyl-3-(2-furyl)-propenal	141.62±2.56	245.49±3.88
	5-Methyl-2-phenyl-2-hexenal	26.31±0.93	10.23±0.87
	Benzeneacetaldehyde, .alpha.-ethylidene-	15.17±0.83	19.22±0.86
	Heptanal	2.98±0.55	-
	2-Octenal, (E)-	208.86±5.56	-
	2-Undecenal	84.14±0.81	5.06±0.75
	Vanillin	-	59.69±1.90
	2-Propenal, 3-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	7.33±0.94	6.29±0.91
Furans	2-Acetyl-5-methylfuran	65.52±0.76	31.26±0.63
	Furan, 2-butyltetrahydro-	-	66.23±2.12
Ketones	Acetoin	4.21±0.15	16.98±0.69
	2(3H)-Furanone, dihydro-5-pentyl-	174.52±3.20	306.76±4.78
	Ethanone, 1-(2-furanyl)-	12.78±1.26	-
	5-Hepten-2-one, 6-methyl-	1.09±0.06	-
	1-Propanone, 1-(2-furanyl)-	40.41±1.12	7.21±0.86
	2,5-Cyclohexadiene-1,4-dione,2,5-dimethyl-	20.39±0.98	-
	trans-Furfurylideneacetone	21.24±0.88	26.28±0.91

	2-Undecanone	20.22±1.57	-
	3,4-dihydroxyphenyl-2-propanone	-	19.23±1.58
	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	-	4.03±0.62
	CH ₃ C(O)OCH(CH ₃)C(O)CH ₃	7.09±0.77	27.18±0.83
Pyrazines	Pyrazine, ethyl-	5.05±0.53	-
	Pyrazine, 2,3-dimethyl-	71.24±0.62	23.15±0.81
	Pyrazine, 3-ethyl-2,5-dimethyl-	3.09±0.30	-
	Pyrazine, tetramethyl-	722.33±5.17	1038.16±11.43
	2,3-Dimethyl-5-n-propylpyrazine	3.07±0.27	-
	2,3-Dimethyl-5-isopentylpyrazine	2.07±0.17	-
	Pyrazine, 2,5-dimethyl-3-propyl-	-	4.23±0.26
	2-Acetyl-3,4,6-trimethylpyrazine	-	1.03±0.19
Others	Oxime-, methoxy-phenyl_	53.39±1.14	50.44±1.10
	1,3-Dioxolane, 2-ethyl-2,4,5-trimethyl-	-	1.01±0.13
	Phenol, 2-methyl-	20.17±0.59	23.21±1.41
	Phenol, 4-ethyl-2-methoxy-	91.86±0.81	68.66±1.17
	Phenol, 2,3,5,6-tetramethyl-	56.49±1.05	-
	1,3-Dioxepane, 2-pentadecyl-	30.31±0.49	221.92±4.89
	Thymol	-	37.42±1.71
	Creosol	146.03±4.26	50.82±1.99
	Disulfide, dimethyl	12.05±0.74	6.08±0.76

Note: "-" not detected by HS-SPME-GC-MS. **Black fonts indicate VFCs with significant differences in aged HBV and SV.**