

**Table S1.** VOCs identified in wheat kernels and wheat beers obtained by them. Compounds are ordered by chemical group and subsequently retention time.

Chemical group	VOCs in wheat kernel	VOCs in wheat beer
Alcohols	1-Butanol, 2-methyl- 1-Pentanol 3-Hexen-1-ol 1-Hexanol 1-Pentanol, 2-ethyl 1-Heptanol 1-Octen-3-ol 5-Hepten-2-ol, 6-methyl 2-Ethyl-1-hexanol Benzyl alcohol 2-Octen-1-ol, (E)- 1-Octanol Phenethyl Alcohol 1-Nonanol 1-Decanol 1-Undecanol 1-Dodecanol 2-Tridecanol 1-Tridecanol 2-Hexadecanol 2-Heptadecanol	1-Propanol, 2-methyl- 1-Butanol, 3-methyl- 1-Butanol, 2-methyl- 2-Ethyl-1-hexanol 1-Octanol Phenethyl Alcohol 1-Decanol
Aldehydes	Butanal, 2-methyl- Pentanal Hexanal 2-Hexenal, (E)- Heptanal 2-Heptenal, (Z)- Benzaldehyde Octanal Phenylacetaldehyde 2-Octenal, (E)- Nonanal 2-Nonenal, (E)- Benzaldehyde, 3-ethyl- Decanal 2,4-Nonadienal, (E,E)- Isophthalaldehyde 4-Oxononanal 2-Decenal, (Z)- Undecanal 2,4-Decadienal, (E,E)- 2-Undecenal Vanillin Dodecanal Tridecanal Tetradecanal Pentadecanal	Nonanal Decanal
Alkanes	Octane, 2-methyl- Undecane Dodecane Tridecane Tetradecane Pentadecane Hexadecane Octadecane	
Alkenes	1-Dodecene 1-Tetradecene 1-Pentadecene 1-Hexadecene	
Benzene derivatives	Toluene	Styrene

Chemical group	VOCs in wheat kernel	VOCs in wheat beer
	Styrene	
Esters	Benzyl Benzoate Methyl hexanoate Ethyl decanoate Diethyl Phthalate Ethyl dodecanoate Tetradecanoic acid, ethyl ester Diisobutyl phthalate Ethyl palmitate	Ethyl acetate 2-Methylpropyl acetate Ethyl butyrate 3-Methylbutyl acetate Ethyl hexanoate Ethyl heptanoate Heptyl acetate Ethyl octanoate Nonyl acetate Ethyl 2-phenylacetate 2-Phenylethyl acetate Ethyl nonanoate Ethyl 9-decenoate Ethyl decanoate Ethyl dodecanoate
Ethers	Ethanol, 2-butoxy- Guaiacol Benzene, 1,2-dimethoxy- Ethanol, 2-(2-butoxyethoxy)- Diphenyl ether	
Ketones	2-Heptanone 5-Hepten-2-one, 6-methyl- 3-Octen-2-one 2,3-Octanedione Acetophenone 3,5-Octadien-2-one, (E,E)- 2-Nonanone 3,5-Nonadien-2-one 3,5-Heptadien-2-one, 6-methyl-, (E)- Isophorone 2-Decanone 3-hepten-2-one, 5-ethyl-6-methyl-, (3E)- 2-Sec-Butylcyclohexanone Ethanone, 1-(3,4-dimethylphenyl)- 2-Undecanone 1,4-Diacetylbenzene 5,9-Undecadien-2-one,6,10-dimethyl- trans- $\beta$ -Ionone 2-tridecanone 2-Pentadecanone 2-Pentadecanone, 6,10, 14-trimethyl- 2-Heptadecanone	2-Nonanone
Lactones	$\gamma$ -Butyrolactone $\gamma$ -Caprolactone $\gamma$ -Octalactone $\gamma$ -Nonalactone Coumarin	
Organic acids	Acetic acid Pentanoic acid Hexanoic acid Heptanoic acid Hexanoic acid, 2-ethyl Octanoic acid Nonanoic acid Decanoic acid Dodecanoic acid Myristic acid n-Hexadecanoic acid	Pentanoic acid Octanoic acid Decanoic acid
Others	Oxime-, methoxy-phenyl- Phenol Furan, 2-pentyl-	2-Methoxy-4-vinylphenol

Chemical group	VOCs in wheat kernel	VOCs in wheat beer
	Benzothiazole	
	2,4-Di-tert-butylphenol	
Terpenes	$\alpha$ -Phellandrene $\alpha$ -Pinene $\alpha$ -Thujene $\beta$ -Pinene $\alpha$ -Terpinene p-Cymene Limonene $\gamma$ -Terpinene cis-Linalool Oxide Camphene Levomenthol $\alpha$ -Terpineol Piperitone Ascaridole $\alpha$ -Cubebene $\alpha$ -Copaene $\beta$ -Bourbonene $\beta$ -Caryophyllene $\beta$ -Gurjunene cis- $\beta$ -Farnesene $\alpha$ -Humulene D-Germacrene $\beta$ -Selinene Valencen $\gamma$ -Cadinene $\delta$ -Cadinene trans-Calamenene Dihydroactinidiolide $\alpha$ -Calacorene Spathulenol $\beta$ -Selinenol Cadalene	$\beta$ -Linalool