Ionization effects on the partitioning behavior of food and beverage aroma compounds between aqueous phases and air and organic matrices

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Abstract

Aroma compounds in the Flavornet database were screened for ionizable functional groups such as carboxylic acids, aliphatic and aromatic amines, phenols, alcohols, and thiols. Of the 738 aroma compounds listed in this database, 101 molecules have ionizable moieties with estimated monomeric aqueous pK_a values ranging between 1.75 and 10.97. pH dependent effective air/water partitioning coefficients ($K_{aw,eff}$) and n-octanol/water partitioning coefficients (D_{ow}) were estimated for all ionizable aroma compounds over the pH range from 0 to 14. The ionizable aroma compounds display a broad range of $K_{aw,eff}$ (1.8×10^{-23} to 6.1 atm M^{-1}) and log D_{ow} (-6.2 to +7.2 units) values. For many aroma compounds, pH dependent ionization will have a significant effect on the $K_{aw,eff}$ and D_{ow}, leading to variations in these physico-chemical properties by up to 11 orders of magnitude over the composite pH range of common foods and beverages. Changes in food and beverage pH affect not only the relative contributions of neutral versus charged forms of ionizable aroma compounds (which directly affects analyte volatility and olfactory reception), but also partitioning between freely dissolved and sorbed forms of the analyte in solution (which indirectly affects analyte volatility).

Keywords: Aroma compounds, Ionization, Air/water partitioning, n-Octanol/water partitioning, Odor threshold, pH dependence

1. Introduction

The partition coefficient between the headspace and the matrix (K_{hm}) represents the equilibrium concentration of an aroma flavor compound in the headspace (C_h) above a product relative to the total concentration of the compound in a food or beverage matrix (C_m; $K_{hm}=C_h/C_m$) (Taylor, 2002). Various factors can influence K_{hm}, including (where relevant) temperature, pH, solution viscosity, emulsion droplet sizes and emulsifier structure, and other components of the matrix that may interact with the analyte of interest (Bohnenstengel et al., 1993; Buttery et al., 1995; Conner et al., 1994a; Conner et al., 1994b; Da Porto and Nicoli, 2002; Giroux et al., 2007; Guyot et al., 1996; Juteau et al., 2004; Lubbers and Guichard, 2003; Morakul et al., 2010; Nahon et al., 2000; Nahon et al., 1998; Roberts et al., 2003; Savary et al., 2006; Steffen and Pawliszyn, 1996; Terta et al., 2006; Whiton and Zoecklein, 2000; Zhang and Pawliszyn, 1993). The role of pH in controlling aroma compound release is complex. Changes in pH not only affect speciation of the analyte between neutral and charged forms, but also affect the physical and chemical nature of the matrix. Proteinaceous components of the matrix may become more aggregated at acidic pH values, reducing their surface area and subsequent capacity to sorb aroma compounds (Leksrisompong et al., 2010). Charges on various small and macromolecular compounds in the matrix may also vary with pH, altering electrostatic interactions and hydrophilic/hydrophobic partitioning behavior between matrix components and aroma compounds (Fares et al., 1998; van Ruth and Villeneuve, 2002). In alcoholic systems, the presence of ethanol generally increases the solubility of volatile flavor compounds, thereby reducing K_{hm}, although the magnitude of this effect depends on analyte hydrophobicity and the ethanol concentration (Athes et al., 2004;

Aznar et al., 2004; Conner et al., 1998; Escalona et al., 1999). One must also recognize that a K_{hm} based analysis of flavor compounds in any system assumes equilibrium conditions, which may not necessarily be relevant for the product being consumed (Doyen et al., 2001; Marin et al., 1999; Tsachaki et al., 2008; Tsachaki et al., 2005; Tsachaki et al., 2005).

A number of aroma compounds also contain ionizable functional groups such as carboxylic acids, aliphatic and aromatic amines, phenols, alcohols, and thiols. Whereas the neutral species of an aroma compound is volatile, and may interact with olfactory receptors, the charged species are non-volatile, and remain in the matrix. Consequently, the pH of a food or beverage matrix and the pK_a values of various moieties on an ionizable aroma compound both define the amount of an analyte present in its neutral volatile form. Despite their fundamental importance in sensory science, few studies have explicitly considered the effects of ionization on the partitioning behavior and odor thresholds of aroma compounds (Guyot et al., 1996; Hartwig and McDaniel, 1995). Two of the most common partitioning constants in general use are the air/water partitioning coefficient ($K°_{aw}$) and the n-octanol/water partitioning coefficient (K_{ow}) (Amoore and Buttery, 1978). Because charged species are not volatile, for ionizable compounds $K°_{aw}$ (which refers to the air/water partitioning behavior when an analyte is present entirely in its neutral form) is replaced by the pH dependent effective air/water partitioning coefficient ($K_{aw,eff}$). Likewise, K_{ow} is the designation for the partitioning behavior of the neutral species, whereas D_{ow} refers to the combined partitioning behavior of all neutral and charged forms of a compound between n-octanol and water, and is also pH dependent (Rayne and Forest, 2010; Wells, 2006). In the current Communication, we investigate a large database of known aroma compounds for

potentially ionizable functional groups, calculate their acidity constants (pK_a) and pH dependent air/water ($K_{aw,eff}$) and octanol-water (D_{ow}) partitioning coefficients, and examine the potential importance of the findings for developing a better theoretical understanding regarding the physico-chemical controls on flavor profiles in foods and beverages.

2. Material and methods

The identities, Chemical Abstracts Service (CAS) registry numbers, molecular weights, and characteristic aromas of compounds were obtained from the online Flavornet database (http://www.flavornet.org/). Monomeric aqueous pK_a values were estimated using the corresponding SPARC software program (http://archemcalc.com/sparc/; September 2009 release w4.5.1522-s4.5.1522) module with the full speciation option for ionizable functional groups, including nitrogen moieties acting as both acids and bases. pH dependent n-octanol/water distribution coefficients (D_{ow}) and effective air/water partitioning coefficients ($\log_{10} K_{aw,eff}$; atm M^{-1}; calculated by SPARC assuming only neutral species are volatile [$K°_{aw}$] and that any charged species predicted to be present at a given pH are not volatile) were calculated using SPARC's "logD" and "Henry(pH)" modules, respectively. Previous work has validated these SPARC modules for the prediction of pK_a, K_{aw}, and D_{ow} values for a wide range of compounds (see, e.g., ref. (Carreira et al., 1994; Goss, 2008b; Goss, 2008a; Hilal et al., 2004; Hilal et al., 1995; Hilal et al., 2007; Rayne, 2009; Rayne and Forest, 2009b; Rayne and Forest, 2009a; Rayne et al., 2009b; Rayne et al., 2009a)).

3. Results and discussion

Of the 738 aroma compounds listed in the Flavornet database, 101 molecules have ionizable functional groups with pK_a values ranging between 1.75 and 10.97 (Table 1 and Figure 1). The compounds chosen also display a broad range of $K_{aw,eff}$ (1.8×10^{-23} to 6.1 atm M^{-1}) and log D_{ow} (-6.2 to +7.2 units) values (Supplementary Materials Tables S1 and S2) and molecular weights (48.1 to 282.5 g mol^{-1}). Estimated $K_{aw,eff}$ values at 0.5 pH intervals and log D_{ow} values at 0.2 pH intervals from pH 0 and 14 for each compound are provided in the Supplementary Materials.

Between typical wine pH values of 2.8 and 4.0, changes in the extent of aroma compound ionization can result in $K_{aw,eff}$ variations of between 0.5 (i.e., two-fold reduction in $K_{aw,eff}$ as the pH is raised from 2.8 to 4.0; benzoic acid) and 15.8 (i.e., almost 16-fold increase in $K_{aw,eff}$ as the pH is raised from 2.8 to 4.0; trimethylamine) (Figure 2(a)). For the pH end members of 2.0 and 12.0, the $K_{aw,eff}$ variations can range from $10^{-10.8}$ (p-coumaric acid) to $10^{+8.9}$ (pyrrolidine) (Figure 2(b)). In other words, for some of these compounds, the $K_{aw,eff}$ can vary by up to 11 orders of magnitude between pH 2.0 and 12.0, either increasing or decreasing (or both trends in different regions of this pH range depending on the pH dependent speciation patterns) due to the acidic or basic nature of the ionizable group(s). By comparison, variability in the volatility of various non-ionizable flavor compounds only decreases by up to about 40% to 70% in the presence of 10% and 20% v/v ethanol, respectively, relative to pure water (Athes et al., 2004; Tsachaki et al., 2008). Similarly, the log D_{ow} can vary between -0.3 units (benzoic acid) and +1.4 units (pyridine) as the pH is raised from 2.8 to 4.0 (Figure 3(a)), and between -6.1 units (benzoic acid) and +3.4

units (o-picoline) as the pH is raised from 2.0 to 12.0 (Figure 3(b)).

Ionization can thus play a significant role in explaining the inherent variability reported for odor thresholds in the literature. For example, it is not uncommon for odor thresholds of aroma compounds in wine (or water, whose pH can vary by up to one unit depending on air temperature and pressure and whether the sample is equilibrated to atmospheric concentrations of carbon dioxide) to be reported with variability in threshold concentrations of up to an order of magnitude. Wine-specific sorption to the unique spectrum of matrix components in different wines will play a significant role in determining the amount of freely dissolved aroma compound able to volatilize and reach olfactory receptors, as will synergistic and antagonistic effects at olfactory receptors between the unique volatile aroma compound mixtures generated from different wines and the inherent differences among sensory participants. However, the varying speciation profiles of ionizable compounds in wines having different pH values will also be important, if not dominant.

For example, based on a reduction in ionization alone (and the associated increase in $K_{aw,eff}$) - with all other wine-specific factors being equivalent - one would expect a 16-fold decrease in the odor threshold concentration of trimethylamine between a wine at pH 2.8 and another wine at pH 4.0 (the typical pH range of wines). In comparison, the odor threshold concentration of benzoic acid would be expected to increase by a factor of two over this pH range between otherwise equivalent wines, due solely to the increased ionization of this aroma compound (and decreased volatility) as the pH is raised. Analogous effects will be evident in other foods and beverages,

particularly where there is either a significant pH variation between different types of products, or within different subsamples of the same product class.

In a similar manner, the partitioning of ionizable compounds between the aqueous and organic matrices of various foods and beverages will also be pH dependent. To use the example of red wine, aroma compounds are known to sorb to and partition into large macromolecular structures present in the wine (e.g., tannins, polysaccharides, and proteins) and/or to solids the wine is in contact with (e.g., oak barrel surfaces, oak chips/staves, lees, fining agents, etc.), and that such partitioning influences the availability of aroma compounds for volatilization (Aronson and Ebeler, 2004; Barrera-Garcia et al., 2006; Chassagne et al., 2005; Dufour and Bayonove, 1999; Garde-Cerdan and Ancin-Azpilicueta, 2006; Perez-Serradilla and Luque de Castro, 2008; Pozo-Bayon and Reineccius, 2009; Ramirez-Ramirez et al., 2004; Ramirez-Ramirez et al., 2001). Analogous sorption of aroma compounds by biopolymers and macromolecules occurs in many other foods and beverages (Belitz et al., 2009; Le Thanh et al., 1992; van Ruth and Villeneuve, 2002). D_{ow} values, or other aqueous/organic solution partitioning coefficients, are often effective used as proxies to describe such sorption behavior. Thus, changes in wine pH affect not only the relative contributions of neutral versus charged forms of ionizable aroma compounds (which directly affects analyte volatility and olfactory reception), but also partitioning between freely dissolved and sorbed forms of the analyte in solution (which indirectly affects analyte volatility).

4. Conclusion

Of 738 aroma compounds listed in the Flavornet database, 101 molecules have ionizable functional groups with estimated monomeric aqueous pK_a values ranging between 1.75 and 10.97. pH dependent ionization of these molecules will have a significant effect on their air/water and n-octanol/water partitioning behavior, leading to variations in these physico-chemical properties by up to 11 orders of magnitude over the composite pH range of common foods and beverages. Changes in food and beverage pH will affect the relative contributions of neutral versus charged forms of ionizable aroma compounds (directly affecting analyte volatility and olfactory reception) as well as partitioning between freely dissolved and sorbed forms of the analyte in solution (indirectly affecting analyte volatility).

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Figure Captions

Figure 1. Frequency histogram of pK_a values for the 101 ionizable aroma compounds in the Flavornet database.

Figure 2. pH dependent effective air/water partitioning coefficients ($K_{aw,eff}$) for (a) benzoic acid (solid line) and trimethylamine (dash-dot-dot line) and (b) p-coumaric acid (solid line) and pyrrolidine (dash-dot-dot line).

Figure 3. pH dependent n-octanol/water partitioning coefficients (D_{ow}) for (a) benzoic acid (solid line) and pyridine (dash-dot-dot line) and (b) o-picoline (solid line).

Table 1. Identities, characteristic aromas, estimated pK_a values, and differences in the effective air/water partitioning coefficient ($K_{aw,eff}$) and n-octanol/water distribution coefficient ($\log_{10} D_{ow}$) between pH values of 2.8→4.0 and 2.0→12.0 of 101 ionizable aroma compounds in the Flavornet database.

					$K_{aw,eff}$		$\log_{10} D_{ow}$	
compound	aroma	CAS-RN	MW (g mol^{-1})	pK_a	ratio (pH 4.0:2.8)	$\log_{10}$ ratio (pH 12.0:2.0)	Δ(pH 2.8→4.0)	ΔpH (2.0→12.0)
trimethylamine	fish	75-50-3	59.11	9.95	15.8	8.0	0.0	2.5
methanethiol	sulfur, gasoline, garlic	74-93-1	48.10	9.90	1.0	-2.1	0.0	-2.1
pyrrolidine	alkaline	123-75-1	71.22	10.97	15.8	8.9	0.0	2.3
propanoic acid	pungent, rancid, soy	79-09-4	74.08	4.75	0.9	-7.3	-0.1	-4.6
butyric acid	rancid, cheese, sweat	107-92-6	88.10	4.75	0.9	-7.3	-0.1	-4.6
acetic acid	sour	64-19-7	60.00	4.77	0.9	-7.2	-0.1	-4.5
methylbutenthiol	amine, smoke	5287-45-6	102.20	9.87	1.0	-2.1	0.0	-2.1
pyridine	rancid	110-86-1	79.10	4.87	14.1	2.7	1.4	2.8
methyl pyrazine	popcorn	109-08-0	94.10	2.14	1.2	0.4	0.2	0.4
isovaleric acid	sweat, acid, rancid	503-74-2	102.10	4.75	0.9	-7.3	-0.1	-4.6
methylfuranthiol	meat	28588-74-1	114.20	6.45	1.0	-5.6	0.0	-5.4
methylbutyric acid	cheese, sweat	116-53-0	102.10	4.72	0.8	-7.3	-0.1	-4.9
dimethylthiazole	rubber, mold	541-58-2	113.20	4.04	9.8	2.0	0.9	1.3
o-picoline	sweat	109-06-8	93.13	5.67	15.5	3.7	1.4	3.4
methyltetrahydrofuranthiol	onion	26548-78-7	118.20	9.25	1.0	-2.8	0.0	-2.8
2,5-dimethyl pyrazine	cocoa, roasted nut, roast beef, medicine	123-32-0	108.14	2.80	1.9	0.9	0.5	0.9
2,6-dimethyl pyrazine	roasted nut, cocoa, roast beef	108-50-9	108.14	2.86	2.0	0.9	0.5	0.9
2-ethyl pyrazine	peanut butter, wood	13925-00-3	108.14	2.13	1.2	0.4	0.2	0.4
caproic acid	sweat	142-62-1	116.10	4.75	0.9	-7.3	-0.1	-4.5
pentanoic acid	sweat	109-52-4	102.10	4.75	0.9	-7.3	-0.1	-4.5
2,3-dimethyl pyrazine	nut, peanut butter, cocoa, meat	5910-89-4	108.14	2.80	1.9	0.9	0.4	0.9
fufuryl mercaptan	coffee, roast	98-02-2	114.00	9.08	1.0	-2.9	0.0	-2.9
acetylpyrroline	nut, roast	85213-22-5	111.14	7.26	15.8	5.3	0.0	0.4
methoxymethylbutanethiol	cat, black currant	94087-83-9	134.24	9.74	1.0	-2.3	0.0	-2.3
ethyl mercaptopropionate	sulfur	19788-49-9	134.20	8.45	1.0	-3.5	0.0	-3.5
4,5-dimethyl thiazole	roast, smoke	3581-91-7	113.18	3.63	5.4	1.6	0.8	1.2
hexanethiol	sulfur	111-31-9	118.10	9.95	1.0	-2.1	0.0	-2.1
2-methyl-4,5-dihydro-3-furanthiol	meat	26486-13-5	116.18	6.35	1.0	-5.7	0.0	-5.4
4-methyl-3-thiazoline	garlic	52558-99-3	101.20	6.66	15.8	4.7	0.0	1.4
2-ethylpyridine	grass	100-71-0	107.15	5.65	15.5	3.7	1.4	3.4
3-mercapto-4-methyl-2-pentanone	black currant	75832-79-0	132.22	9.07	1.0	-2.9	0.0	-2.9
3-mercaptothiophene	cooked meat	7774-73-4	116.21	5.08	0.9	-6.9	0.0	-5.7
2,5-dimethyl-3-furanthiol	meat	55764-23-3	128.20	6.71	1.0	-5.3	0.0	-5.2
3-mercapto-3-methyl-1-butanol	meat broth	34300-94-2	118.20	9.84	1.0	-2.2	0.0	-2.2
2-ethyl-5-methyl pyrazine	fruit, sweet	13360-64-0	122.10	2.79	1.9	0.9	0.4	0.9
2,4,5-trimethylthiazole	earth	13623-11-5	127.00	4.74	11.7	2.8	0.6	1.3
2,3,5-trimethylpyrazine	roast, potato, must	14667-55-1	122.10	3.49	4.5	1.5	0.9	1.5
2-acetylpyridine	popcorn	1122-62-9	121.10	3.24	3.2	1.3	0.7	1.3
5-methyl-2-furfurylthiol	sulfur, roast	59303-05-8	128.19	9.29	1.0	-2.7	0.0	-2.7
2-acetylthiazole	roast, nut, sulfur	24295-03-2	127.00	2.42	1.4	0.6	0.2	0.5
2-propionyl-1-pyrroline	roast	133447-37-7	125.17	7.27	15.8	5.3	0.0	0.4
2-acetyl-1,4,5,6-tetrahydropyridine	caramel	25343-57-1	125.17	5.31	15.2	3.3	1.2	2.7

2-ethyl-6-methylpyrazine	sweat	33504-66-4	122.17	2.85	2.0	0.9	0.5	0.9
2-isobutylthiazole	tomato leaf, green	18640-74-9	141.24	4.02	12.0	2.0	0.8	1.2
4-mercapto-4-methyl-2-pentanone	box tree	19872-52-7	132.22	9.99	1.0	-2.0	0.0	-2.0
2-methyl-3-ethylpyrazine	roast	15707-23-0	122.10	2.79	1.9	0.9	0.4	0.9
2-methyl-3-thiophenethiol	medicine	2527-76-6	130.23	5.59	0.9	-6.4	0.0	-5.6
5-isopropyl-2-methylpyrazine	sweat	13925-05-8	136.19	2.78	1.6	0.8	0.4	0.9
2-methoxy-3,6-dimethylpyrazine	earth	19846-22-1	138.17	2.60	1.6	0.7	0.3	0.7
5-ethyl-2,4-dimethylthiazole	earth	38205-61-7	141.10	4.74	13.3	2.7	0.5	1.2
2,5-dimethyl-3-ethylpyrazine	potato, roast	13360-65-1	136.10	3.48	4.4	1.5	0.9	1.5
thenylthiol	sulfur	6258-63-5	130.23	8.97	1.0	-3.0	0.0	-3.0
2-ethyl-3,5-dimethylpyrazine	potato	13925-07-0	136.20	3.48	4.5	1.5	0.9	1.5
2,3-dimethyl-6-ethylpyrazine	burnt, popcorn	15707-34-3	136.10	3.48	4.4	1.5	0.9	1.5
2-ethyl-3,5-dimethylpyrazine	roast	13925-07-0	136.20	3.48	4.5	1.5	0.9	1.5
2-isopropyl-3-methoxypyrazine	pea, earth	25773-40-4	152.10	1.94	1.1	0.3	0.1	0.3
2-ethenyl-3,5-dimethylpyrazine	earth	157615-33-3	205.20	2.88	2.0	0.9	0.5	0.9
2-acetyl-2-thiazoline	roast, popcorn	29926-41-8	129.20	5.56	15.4	3.6	0.3	1.6
2-acetyl-3,4,5,6-tetrahydropyridine	caramel	27300-27-2	125.17	7.25	15.8	5.3	0.0	0.4
4-mercapto-4-methyl-2-pentanol	flower, lemon	31539-84-1	134.24	9.84	1.0	-2.2	0.0	-2.2
5-methyl-5(H)-cyclopentapyrazine	roast	65128-99-6	132.16	2.83	1.9	0.9	0.5	0.9
3,5-diethyl-2-methylpyrazine	baked	18138-05-1	150.22	3.46	4.3	1.5	0.9	1.5
2,3-diethyl-5-methylpyrazine	potato, meat, roast	18138-04-0	150.10	3.47	4.4	1.5	0.9	1.5
2-sec-butyl-3-methoxypyrazine	carrot, earth	24168-70-5	166.22	1.89	1.1	0.3	0.1	0.3
2-phenylethylthiol	rubber	4410-99-5	138.23	9.73	1.0	-2.3	0.0	-2.3
2-ethenyl-3-ethyl-5-methylpyrazine	earth	181589-32-2	148.21	2.87	2.0	0.9	0.5	0.9
2-pentylpyridine	fat	2294-76-0	149.24	5.65	15.5	3.7	1.4	3.4
2-isobutyl-3-methoxypyrazine	earth, spice, green pepper	24683-00-9	166.10	1.96	1.1	0.3	0.1	0.3
isobutyric acid	rancid, butter, cheese	79-31-2	88.10	4.72	0.8	-7.3	-0.1	-4.7
benzothiazole	gasoline, rubber	95-16-9	135.00	1.75	1.1	0.2	0.1	0.2
3-mercapto-1-hexanol-1-acetate	box tree	136954-20-6	176.28	9.48	1.0	-2.5	0.0	-2.5
6,7-dihydro-5-methyl-5H-cyclopentapyrazine	roast, nut	23747-48-0	134.18	2.47	1.4	0.6	0.3	0.6
phenylacetic acid	honey, flower	103-82-2	136.10	4.44	0.7	-7.6	-0.1	-4.7
4-methyl-5-hydroxyethyl-thiazole	sulfur	137-00-8	143.00	3.35	3.7	1.4	0.7	1.1
o-aminoacetophenone	foxy, sweet	551-93-9	135.10	2.20	1.2	0.4	0.2	0.4
nonanoic acid	green, fat	112-05-0	158.10	4.75	0.9	-7.3	-0.1	-4.4
benzoic acid	urine	65-85-0	122.00	4.03	0.5	-8.0	-0.3	-6.1
octanoic acid	sweat, cheese	124-07-2	144.10	4.75	0.9	-7.3	-0.1	-4.4
p-menthenethiol	grapefruit	71159-90-5	170.32	10.17	1.0	-1.8	0.0	-1.8
methyl quinoxaline	roast, nut, fruit	7251-61-8	144.17	1.87	1.1	0.2	0.1	0.2
2-isopentyl-3,6-dimethyl pyrazine	fruit	18433-98-2	178.28	3.48	4.4	1.5	0.9	1.5
hydrocinnamic acid	balsamic	501-52-0	150.17	4.60	0.8	-7.4	-0.1	-4.5
4-methylthiazole	roasted meat	693-95-8	99.16	2.94	2.0	1.0	0.5	0.9
methyl anthranilate	honey, flower	134-20-3	151.10	2.04	1.2	0.3	0.1	0.3
decanoic acid	rancid, fat	334-48-5	172.10	4.75	0.9	-7.3	-0.1	-4.4
cinnamic acid	honey	140-10-3	148.10	4.11	0.6	-7.9	-0.2	-2.9
p-coumaric acid	balsamic	501-98-4	164.16	4.33, 8.83	0.7	-10.8	-0.2	-6.1
undecylic acid	oil	112-37-8	186.29	4.75	0.9	-7.3	-0.1	-4.3
(E)-2-hexenoic acid	must, fat	13419-69-7	114.14	4.31	0.7	-7.7	-0.2	-3.1

oleic acid	fat	112-80-1	282.47	4.74	0.9	-7.3	-0.1	-4.2
lauric acid	metal	143-07-7	200.30	4.75	0.9	-7.3	-0.1	-4.3
phenol	phenol	108-95-2	94.11	9.91	1.0	-2.1	0.0	-2.1
guaiacol	smoke, sweet, medicine	90-05-1	124.14	9.85	1.0	-2.1	0.0	-2.2
p-cresol	medicine, phenol, smoke	106-44-5	108.10	10.25	1.0	-1.8	0.0	-1.8
m-cresol	fecal, plastic	108-39-4	108.14	10.07	1.0	-1.9	0.0	-1.9
3-ethylphenol	must	620-17-7	122.17	10.07	1.0	-1.9	0.0	-1.9
o-cresol	phenol	95-48-7	108.10	10.32	1.0	-1.7	0.0	-1.7
p-vinylguaiacol	clove, curry	7786-61-0	150.18	9.35	1.0	-2.6	0.0	-2.7
4-propyl-guaiacol	phenol	2785-87-7	166.22	10.19	1.0	-1.8	0.0	-1.8
syringol	medicine, phenol, smoke	91-10-1	154.16	9.23	1.0	-2.8	0.0	-2.8
4-vinylphenol	almond shell	2628-17-3	120.15	9.40	1.0	-2.6	0.0	-2.6

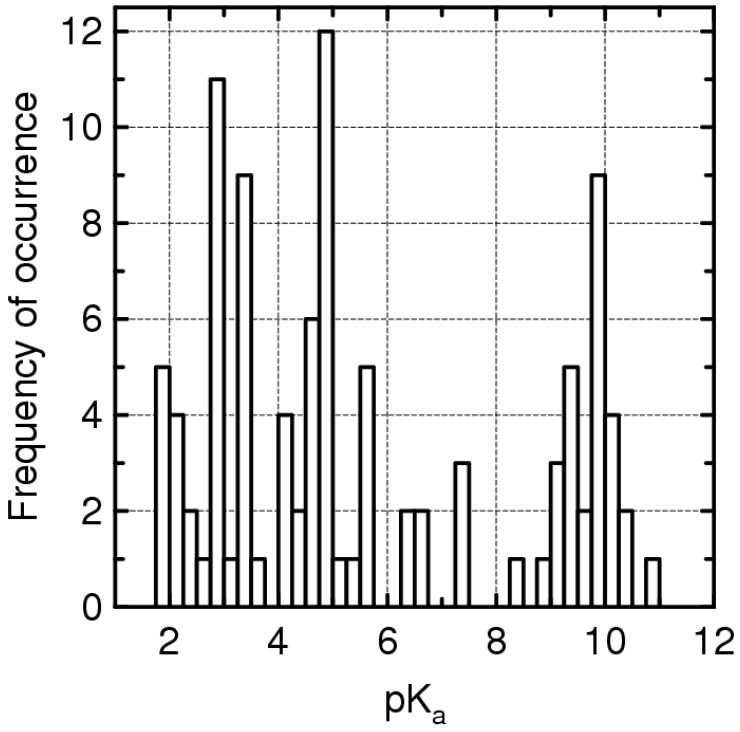

Figure 1.

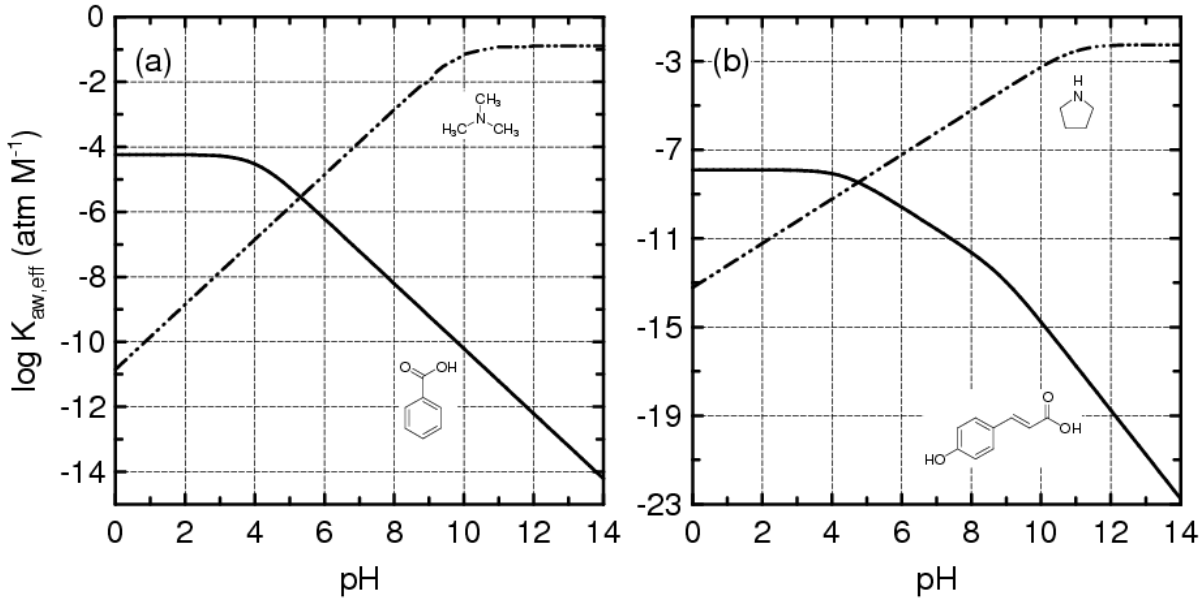
(a)
(b)
log $K_{aw,eff}$ (atm M^{-1})
pH
pH
0
-2
-4
-6
-8
-10
-12
-14
-3
-7
-11
-15
-19
-23
0
2
4
6
8
10
12
14
CH3
H3C
N
CH3
O
OH
H
N
HO
O
OH

Figure 2.

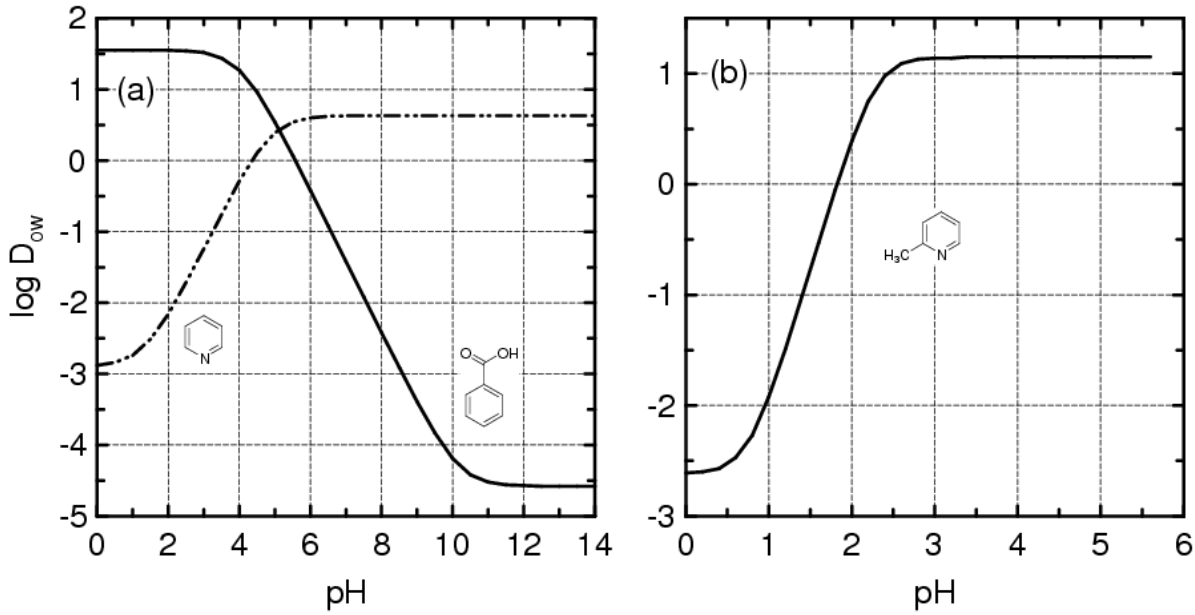

Figure 3.

Supplementary Material

Ionization effects on the partitioning behavior of food and beverage aroma compounds between aqueous phases and air and organic matrices

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Table S1a. SPARC estimated pH dependent effective air/water partitioning coefficients ($K_{aw,eff}$; atm M^{-1}) for ionizable aroma compounds from the Flavornet database.

pH	0.0	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8	2.0	2.2	2.4	2.6	2.8	3.0	3.2	3.4	3.6	3.8
trimethylamine	1.41E-11	2.24E-11	3.55E-11	5.63E-11	8.93E-11	1.41E-10	2.24E-10	3.55E-10	5.63E-10	8.93E-10	1.41E-09	2.24E-09	3.55E-09	5.63E-09	8.93E-09	1.41E-08	2.24E-08	3.55E-08	5.63E-08	8.93E-08
methanethiol	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00
pyrrolidine	6.02E-14	9.54E-14	1.51E-13	2.40E-13	3.80E-13	6.02E-13	9.54E-13	1.51E-12	2.40E-12	3.80E-12	6.02E-12	9.54E-12	1.51E-11	2.40E-11	3.80E-11	6.02E-11	9.54E-11	1.51E-10	2.40E-10	3.80E-10
propanoic acid	1.28E-04	1.28E-04	1.28E-04	1.28E-04	1.28E-04	1.28E-04	1.28E-04	1.28E-04	1.28E-04	1.27E-04	1.27E-04	1.27E-04	1.27E-04	1.27E-04	1.26E-04	1.25E-04	1.24E-04	1.22E-04	1.19E-04	1.15E-04
butyric acid	2.33E-04	2.33E-04	2.33E-04	2.33E-04	2.33E-04	2.33E-04	2.33E-04	2.33E-04	2.33E-04	2.33E-04	2.32E-04	2.32E-04	2.32E-04	2.31E-04	2.30E-04	2.29E-04	2.26E-04	2.23E-04	2.17E-04	2.09E-04
acetic acid	7.23E-05	7.23E-05	7.23E-05	7.23E-05	7.23E-05	7.23E-05	7.23E-05	7.23E-05	7.23E-05	7.22E-05	7.22E-05	7.21E-05	7.20E-05	7.18E-05	7.16E-05	7.11E-05	7.04E-05	6.94E-05	6.78E-05	6.54E-05
methylbutenthiol	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01
pyridine	1.88E-07	2.97E-07	4.71E-07	7.46E-07	1.18E-06	1.87E-06	2.97E-06	4.71E-06	7.46E-06	1.18E-05	1.87E-05	2.97E-05	4.69E-05	7.43E-05	1.17E-04	1.85E-04	2.91E-04	4.56E-04	7.09E-04	1.09E-03
methyl pyrazine	1.97E-05	3.12E-05	4.91E-05	7.70E-05	1.20E-04	1.86E-04	2.83E-04	4.23E-04	6.16E-04	8.64E-04	1.16E-03	1.48E-03	1.78E-03	2.05E-03	2.27E-03	2.43E-03	2.55E-03	2.63E-03	2.68E-03	2.71E-03
isovaleric acid	3.51E-04	3.51E-04	3.51E-04	3.51E-04	3.51E-04	3.51E-04	3.51E-04	3.51E-04	3.51E-04	3.51E-04	3.51E-04	3.50E-04	3.50E-04	3.49E-04	3.48E-04	3.45E-04	3.42E-04	3.36E-04	3.28E-04	3.16E-04
methylfuranthiol	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02
methylbutyric acid	6.60E-04	6.60E-04	6.60E-04	6.60E-04	6.60E-04	6.60E-04	6.60E-04	6.60E-04	6.59E-04	6.59E-04	6.59E-04	6.58E-04	6.57E-04	6.55E-04	6.52E-04	6.47E-04	6.40E-04	6.30E-04	6.13E-04	5.89E-04
dimethylthiazole	6.87E-06	1.09E-05	1.73E-05	2.74E-05	4.34E-05	6.87E-05	1.09E-04	1.72E-04	2.73E-04	4.31E-04	6.81E-04	1.07E-03	1.69E-03	2.64E-03	4.10E-03	6.30E-03	9.51E-03	1.00E-02	2.00E-02	3.00E-02
o-picoline	5.81E-08	9.20E-08	1.46E-07	2.31E-07	3.66E-07	5.81E-07	9.20E-07	1.46E-06	2.31E-06	3.66E-06	5.81E-06	9.20E-06	1.46E-05	2.31E-05	3.66E-05	5.79E-05	9.17E-05	1.45E-04	2.29E-04	3.61E-04
methyltetrahydrofuranthiol	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03
2,5-dimethyl pyrazine	6.41E-06	1.01E-05	1.61E-05	2.54E-05	4.01E-05	6.32E-05	9.93E-05	1.55E-04	2.40E-04	3.68E-04	5.54E-04	8.13E-04	1.15E-03	1.57E-03	2.03E-03	2.48E-03	2.90E-03	3.24E-03	3.50E-03	3.68E-03
2,6-dimethyl pyrazine	3.12E-06	4.94E-06	7.83E-06	1.24E-05	1.96E-05	3.09E-05	4.85E-05	7.60E-05	1.18E-04	1.82E-04	2.75E-04	4.07E-04	5.85E-04	8.06E-04	1.06E-03	1.32E-03	1.57E-03	1.77E-03	1.93E-03	2.05E-03
2-ethyl pyrazine	3.82E-05	6.03E-05	9.49E-05	1.49E-04	2.32E-04	3.58E-04	5.46E-04	8.15E-04	1.18E-03	1.65E-03	2.21E-03	2.81E-03	3.38E-03	3.88E-03	4.28E-03	4.58E-03	4.79E-03	4.94E-03	5.03E-03	5.09E-03
caproic acid	4.72E-04	4.72E-04	4.72E-04	4.72E-04	4.72E-04	4.72E-04	4.72E-04	4.72E-04	4.72E-04	4.71E-04	4.71E-04	4.71E-04	4.70E-04	4.68E-04	4.67E-04	4.64E-04	4.59E-04	4.52E-04	4.40E-04	4.24E-04
pentanoic acid	3.46E-04	3.46E-04	3.46E-04	3.46E-04	3.46E-04	3.46E-04	3.46E-04	3.46E-04	3.46E-04	3.46E-04	3.46E-04	3.45E-04	3.45E-04	3.44E-04	3.43E-04	3.40E-04	3.37E-04	3.32E-04	3.23E-04	3.11E-04
2,3-dimethyl pyrazine	5.26E-06	8.33E-06	1.32E-05	2.09E-05	3.29E-05	5.19E-05	8.15E-05	1.27E-04	1.97E-04	3.02E-04	4.55E-04	6.68E-04	9.47E-04	1.29E-03	1.66E-03	2.04E-03	2.38E-03	2.66E-03	2.87E-03	3.02E-03
fufuryl mercaptan	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02
acetylpyrroline	1.43E-11	2.27E-11	3.60E-11	5.70E-11	9.04E-11	1.43E-10	2.27E-10	3.60E-10	5.70E-10	9.04E-10	1.43E-09	2.27E-09	3.60E-09	5.70E-09	9.04E-09	1.43E-08	2.27E-08	3.60E-08	5.70E-08	9.04E-08
methoxymethylbutanethiol	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02
ethyl mercaptopropionate	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02
4,5-dimethyl thiazole	1.68E-05	2.67E-05	4.23E-05	6.70E-05	1.06E-04	1.68E-04	2.66E-04	4.21E-04	6.64E-04	1.05E-03	1.65E-03	2.57E-03	4.00E-03	6.13E-03	9.26E-03	1.00E-02	2.00E-02	3.00E-02	3.00E-02	4.00E-02
hexanethiol	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00
2-methyl-4,5-dihydro-3-furanthiol	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02
4-methyl-3-thiazoline	1.04E-09	1.65E-09	2.61E-09	4.14E-09	6.57E-09	1.04E-08	1.65E-08	2.61E-08	4.14E-08	6.57E-08	1.04E-07	1.65E-07	2.61E-07	4.14E-07	6.57E-07	1.04E-06	1.65E-06	2.61E-06	4.14E-06	6.56E-06
2-ethylpyridine	8.72E-08	1.38E-07	2.19E-07	3.47E-07	5.50E-07	8.72E-07	1.38E-06	2.19E-06	3.47E-06	5.50E-06	8.71E-06	1.38E-05	2.19E-05	3.47E-05	5.49E-05	8.70E-05	1.38E-04	2.18E-04	3.44E-04	5.42E-04
3-mercapto-4-methyl-2-pentanone	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02
3-mercaptothiophene	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.70E-01
2,5-dimethyl-3-furanthiol	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02
3-mercapto-3-methyl-1-butanol	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03
2-ethyl-5-methyl pyrazine	1.13E-05	1.80E-05	2.84E-05	4.49E-05	7.10E-05	1.12E-04	1.76E-04	2.74E-04	4.25E-04	6.50E-04	9.78E-04	1.43E-03	2.03E-03	2.75E-03	3.54E-03	4.33E-03	5.04E-03	5.62E-03	6.06E-03	6.38E-03
2,4,5-trimethylthiazole	1.38E-06	2.18E-06	3.46E-06	5.48E-06	8.68E-06	1.38E-05	2.18E-05	3.45E-05	5.47E-05	8.67E-05	1.37E-04	2.17E-04	3.44E-04	5.44E-04	8.58E-04	1.35E-03	2.12E-03	3.30E-03	5.11E-03	7.79E-03
2,3,5-trimethylpyrazine	7.44E-07	1.18E-06	1.87E-06	2.96E-06	4.70E-06	7.44E-06	1.18E-05	1.86E-05	2.93E-05	4.61E-05	7.23E-05	1.12E-04	1.73E-04	2.63E-04	3.91E-04	5.63E-04	7.81E-04	1.03E-03	1.30E-03	1.54E-03
2-acetylpyridine	4.92E-08	7.80E-08	1.24E-07	1.96E-07	3.10E-07	4.90E-07	7.73E-07	1.22E-06	1.92E-06	3.00E-06	4.66E-06	7.15E-06	1.08E-05	1.59E-05	2.28E-05	3.12E-05	4.07E-05	5.04E-05	5.94E-05	6.69E-05
5-methyl-2-furfurylthiol	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02
2-acetylthiazole	2.70E-07	4.26E-07	6.74E-07	1.06E-06	1.67E-06	2.61E-06	4.05E-06	6.20E-06	9.35E-06	1.38E-05	1.96E-05	2.67E-05	3.47E-05	4.28E-05	5.01E-05	5.62E-05	6.08E-05	6.42E-05	6.65E-05	6.80E-05
2-propionyl-1-pyrroline	3.09E-11	4.90E-11	7.76E-11	1.23E-10	1.95E-10	3.09E-10	4.90E-10	7.76E-10	1.23E-09	1.95E-09	3.09E-09	4.90E-09	7.76E-09	1.23E-08	1.95E-08	3.09E-08	4.90E-08	7.76E-08	1.23E-07	1.95E-07
2-acetyl-1,4,5,6-tetrahydropyridine	2.75E-08	4.36E-08	6.92E-08	1.10E-07	1.74E-07	2.75E-07	4.36E-07	6.92E-07	1.10E-06	1.74E-06	2.75E-06	4.36E-06	6.91E-06	1.09E-05	1.73E-05	2.74E-05	4.33E-05	6.83E-05	1.08E-04	1.69E-04
2-ethyl-6-methylpyrazine	5.07E-06	8.03E-06	1.27E-05	2.01E-05	3.18E-05	5.01E-05	7.88E-05	1.23E-04	1.92E-04	2.94E-04	4.45E-04	6.58E-04	9.42E-04	1.29E-03	1.69E-03	2.10E-03	2.48E-03	2.80E-03	3.05E-03	3.23E-03
2-isobutylthiazole	2.35E-05	3.73E-05	5.91E-05	9.36E-05	1.48E-04	2.35E-04	3.72E-04	5.90E-04	9.33E-04	1.48E-03	2.33E-03	3.67E-03	5.77E-03	9.03E-03	1.00E-02	2.00E-02	3.00E-02	5.00E-02	7.00E-02	9.00E-02
4-mercapto-4-methyl-2-pentanone	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02
2-methyl-3-ethylpyrazine	9.21E-06	1.46E-05	2.31E-05	3.65E-05	5.77E-05	9.08E-05	1.43E-04	2.23E-04	3.45E-04	5.28E-04	7.94E-04	1.16E-03	1.65E-03	2.23E-03	2.88E-03	3.52E-03	4.09E-03	4.57E-03	4.92E-03	5.18E-03
2-methyl-3-thiophenethiol	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01
5-isopropyl-2-methylpyrazine	2.06E-05	3.27E-05	5.18E-05	8.18E-05	1.29E-04	2.04E-04	3.20E-04	4.99E-04	7.73E-04	1.18E-03	1.77E-03	2.60E-03	3.67E-03	4.96E-03	6.37E-03	7.77E-03	9.02E-03	1.00E-02	1.00E-02	1.00E-02
2-methoxy-3,6-dimethylpyrazine	1.42E-07	2.25E-07	3.56E-07	5.63E-07	8.87E-07	1.39E-06	2.18E-06	3.37E-06	5.17E-06	7.78E-06	1.14E-05	1.62E-05	2.20E-05	2.85E-05	3.49E-05	4.07E-05	4.55E-05	4.92E-05	5.18E-05	5.36E-05
5-ethyl-2,4-dimethylthiazole	2.40E-06	3.81E-06	6.04E-06	9.57E-06	1.52E-05	2.40E-05	3.81E-05	6.03E-05	9.56E-05	1.51E-04	2.40E-04	3.80E-04	6.01E-04	9.50E-04	1.50E-03	2.36E-03	3.70E-03	5.77E-03	8.92E-03	1.00E-02
2,5-dimethyl-3-ethylpyrazine	1.12E-06	1.78E-06	2.83E-06	4.48E-06	7.10E-06	1.12E-05	1.78E-05	2.81E-05	4.43E-05	6.97E-05	1.09E-04	1.70E-04	2.61E-04	3.96E-04	5.88E-04	8.45E-04	1.17E-03	1.54E-03	1.93E-03	2.29E-03
thenylthiol	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01
2-ethyl-3,5-dimethylpyrazine	1.25E-06	1.99E-06	3.15E-06	4.99E-06	7.90E-06	1.25E-05	1.98E-05	3.13E-05	4.93E-05	7.76E-05	1.22E-04	1.89E-04	2.91E-04	4.42E-04	6.56E-04	9.44E-04	1.31E-03	1.72E-03	2.16E-03	2.57E-03
2,3-dimethyl-6-ethylpyrazine	1.14E-06	1.81E-06	2.86E-06	4.54E-06	7.19E-06	1.14E-05	1.80E-05	2.85E-05	4.49E-05	7.06E-05	1.11E-04	1.72E-04	2.65E-04	4.01E-04	5.95E-04	8.56E-04	1.18E-03	1.56E-03	1.95E-03	2.32E-03
2-ethyl-3,5-dimethylpyrazine	1.25E-06	1.99E-06	3.15E-06	4.99E-06	7.90E-06	1.25E-05	1.98E-05	3.13E-05	4.93E-05	7.76E-05	1.22E-04	1.89E-04	2.91E-04	4.42E-04	6.56E-04	9.44E-04	1.31E-03	1.72E-03	2.16E-03	2.57E-03
2-isopropyl-3-methoxypyrazine	5.42E-06	8.53E-06	1.34E-05	2.09E-05	3.23E-05	4.92E-05	7.36E-05	1.07E-04	1.50E-04	2.01E-04	2.56E-04	3.10E-04	3.57E-04	3.94E-04	4.22E-04	4.42E-04	4.56E-04	4.65E-04	4.71E-04	4.75E-04

2-ethenyl-3,5-dimethylpyrazine	3.30E-06	5.23E-06	8.29E-06	1.31E-05	2.07E-05	3.27E-05	5.14E-05	8.05E-05	1.25E-04	1.93E-04	2.93E-04	4.34E-04	6.25E-04	8.65E-04	1.14E-03	1.43E-03	1.70E-03	1.93E-03	2.11E-03	2.24E-03
2-acetyl-2-thiazoline	4.74E-11	7.52E-11	1.19E-10	1.89E-10	2.99E-10	4.74E-10	7.52E-10	1.19E-09	1.89E-09	2.99E-09	4.74E-09	7.51E-09	1.19E-08	1.89E-08	2.99E-08	4.73E-08	7.48E-08	1.18E-07	1.87E-07	2.94E-07
2-acetyl-3,4,5,6-tetrahydropyridine	8.61E-11	1.36E-10	2.16E-10	3.43E-10	5.43E-10	8.61E-10	1.36E-09	2.16E-09	3.43E-09	5.43E-09	8.61E-09	1.36E-08	2.16E-08	3.43E-08	5.43E-08	8.61E-08	1.36E-07	2.16E-07	3.43E-07	5.43E-07
4-mercapto-4-methyl-2-pentanol	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03
5-methyl-5(H)-cyclopentapyrazine	1.31E-06	2.08E-06	3.29E-06	5.20E-06	8.21E-06	1.29E-05	2.03E-05	3.18E-05	4.94E-05	7.58E-05	1.14E-04	1.69E-04	2.41E-04	3.29E-04	4.29E-04	5.30E-04	6.23E-04	7.00E-04	7.60E-04	8.03E-04
3,5-diethyl-2-methylpyrazine	2.18E-06	3.46E-06	5.48E-06	8.69E-06	1.38E-05	2.18E-05	3.45E-05	5.45E-05	8.59E-05	1.35E-04	2.11E-04	3.29E-04	5.06E-04	7.66E-04	1.13E-03	1.63E-03	2.24E-03	2.94E-03	3.67E-03	4.35E-03
2,3-diethyl-5-methylpyrazine	2.32E-06	3.68E-06	5.84E-06	9.25E-06	1.47E-05	2.32E-05	3.67E-05	5.80E-05	9.15E-05	1.44E-04	2.25E-04	3.50E-04	5.39E-04	8.17E-04	1.21E-03	1.74E-03	2.40E-03	3.15E-03	3.94E-03	4.67E-03
2-sec-butyl-3-methoxypyrazine	7.27E-06	1.14E-05	1.79E-05	2.79E-05	4.30E-05	6.53E-05	9.72E-05	1.40E-04	1.95E-04	2.58E-04	3.25E-04	3.88E-04	4.42E-04	4.85E-04	5.17E-04	5.39E-04	5.54E-04	5.64E-04	5.70E-04	5.74E-04
2-phenylethylthiol	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01
2-ethenyl-3-ethyl-5-methylpyrazine	5.08E-06	8.04E-06	1.27E-05	2.01E-05	3.18E-05	5.02E-05	7.89E-05	1.24E-04	1.92E-04	2.96E-04	4.48E-04	6.63E-04	9.52E-04	1.31E-03	1.73E-03	2.15E-03	2.55E-03	2.89E-03	3.15E-03	3.34E-03
2-pentylpyridine	1.74E-07	2.75E-07	4.36E-07	6.91E-07	1.09E-06	1.74E-06	2.75E-06	4.36E-06	6.91E-06	1.09E-05	1.73E-05	2.75E-05	4.36E-05	6.90E-05	1.09E-04	1.73E-04	2.74E-04	4.33E-04	6.85E-04	1.08E-03
2-isobutyl-3-methoxypyrazine	5.97E-06	9.41E-06	1.48E-05	2.31E-05	3.57E-05	5.45E-05	8.18E-05	1.19E-04	1.68E-04	2.27E-04	2.91E-04	3.54E-04	4.10E-04	4.55E-04	4.89E-04	5.14E-04	5.30E-04	5.41E-04	5.49E-04	5.53E-04
isobutyric acid	4.16E-04	4.16E-04	4.16E-04	4.16E-04	4.16E-04	4.16E-04	4.16E-04	4.16E-04	4.16E-04	4.16E-04	4.16E-04	4.15E-04	4.14E-04	4.13E-04	4.11E-04	4.09E-04	4.04E-04	3.97E-04	3.87E-04	3.71E-04
benzothiazole	1.62E-05	2.55E-05	3.97E-05	6.15E-05	9.38E-05	1.41E-04	2.05E-04	2.88E-04	3.87E-04	4.94E-04	5.99E-04	6.92E-04	7.66E-04	8.22E-04	8.62E-04	8.89E-04	9.07E-04	9.19E-04	9.27E-04	9.31E-04
3-mercapto-1-hexanol-1-acetate	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02
6,7-dihydro-5-methyl-5H-cyclopentapyrazine	5.77E-06	9.13E-06	1.44E-05	2.28E-05	3.58E-05	5.60E-05	8.71E-05	1.34E-04	2.03E-04	3.01E-04	4.32E-04	5.95E-04	7.83E-04	9.76E-04	1.16E-03	1.31E-03	1.43E-03	1.52E-03	1.58E-03	1.62E-03
phenylacetic acid	8.76E-06	8.76E-06	8.76E-06	8.76E-06	8.76E-06	8.76E-06	8.75E-06	8.75E-06	8.75E-06	8.74E-06	8.73E-06	8.71E-06	8.68E-06	8.63E-06	8.56E-06	8.45E-06	8.28E-06	8.02E-06	7.65E-06	7.12E-06
4-methyl-5-hydroxyethyl-thiazole	7.95E-09	1.26E-08	1.99E-08	3.16E-08	5.00E-08	7.92E-08	1.25E-07	1.97E-07	3.11E-07	4.88E-07	7.61E-07	1.18E-06	1.80E-06	2.69E-06	3.91E-06	5.50E-06	7.38E-06	9.41E-06	1.14E-05	1.31E-05
o-aminoacetophenone	3.20E-06	5.06E-06	7.97E-06	1.25E-05	1.96E-05	3.03E-05	4.65E-05	6.99E-05	1.03E-04	1.46E-04	1.98E-04	2.56E-04	3.15E-04	3.67E-04	4.11E-04	4.44E-04	4.68E-04	4.84E-04	4.95E-04	5.02E-04
nonanoic acid	1.29E-03	1.29E-03	1.29E-03	1.29E-03	1.29E-03	1.29E-03	1.29E-03	1.29E-03	1.29E-03	1.29E-03	1.29E-03	1.29E-03	1.29E-03	1.28E-03	1.28E-03	1.27E-03	1.26E-03	1.24E-03	1.21E-03	1.16E-03
benzoic acid	5.76E-05	5.76E-05	5.76E-05	5.76E-05	5.76E-05	5.76E-05	5.76E-05	5.75E-05	5.74E-05	5.73E-05	5.71E-05	5.68E-05	5.63E-05	5.56E-05	5.44E-05	5.27E-05	5.02E-05	4.66E-05	4.20E-05	3.62E-05
octanoic acid	8.47E-04	8.47E-04	8.47E-04	8.47E-04	8.47E-04	8.47E-04	8.47E-04	8.47E-04	8.47E-04	8.47E-04	8.46E-04	8.45E-04	8.44E-04	8.41E-04	8.38E-04	8.33E-04	8.24E-04	8.11E-04	7.91E-04	7.61E-04
p-menthenethiol	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00
methyl quinoxaline	5.72E-06	9.00E-06	1.41E-05	2.19E-05	3.37E-05	5.11E-05	7.58E-05	1.09E-04	1.50E-04	1.98E-04	2.48E-04	2.94E-04	3.33E-04	3.64E-04	3.87E-04	4.02E-04	4.13E-04	4.20E-04	4.24E-04	4.27E-04
2-isopentyl-3,6-dimethyl pyrazine	2.03E-06	3.22E-06	5.11E-06	8.09E-06	1.28E-05	2.03E-05	3.21E-05	5.07E-05	8.00E-05	1.26E-04	1.97E-04	3.07E-04	4.72E-04	7.15E-04	1.06E-03	1.53E-03	2.11E-03	2.78E-03	3.48E-03	4.13E-03
hydrocinnamic acid	1.04E-05	1.04E-05	1.04E-05	1.04E-05	1.04E-05	1.04E-05	1.04E-05	1.04E-05	1.04E-05	1.04E-05	1.04E-05	1.04E-05	1.03E-05	1.03E-05	1.02E-05	1.01E-05	1.00E-05	9.78E-06	9.45E-06	8.97E-06
4-methylthiazole	6.87E-05	1.09E-04	1.72E-04	2.73E-04	4.31E-04	6.80E-04	1.07E-03	1.68E-03	2.62E-03	4.05E-03	6.18E-03	9.23E-03	1.00E-02	2.00E-02	3.00E-02	3.00E-02	4.00E-02	4.00E-02	5.00E-02	5.00E-02
methyl anthranilate	3.56E-06	5.61E-06	8.82E-06	1.38E-05	2.14E-05	3.29E-05	4.97E-05	7.34E-05	1.05E-04	1.44E-04	1.88E-04	2.33E-04	2.74E-04	3.08E-04	3.35E-04	3.54E-04	3.68E-04	3.77E-04	3.83E-04	3.86E-04
decanoic acid	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.64E-03	1.63E-03	1.62E-03	1.61E-03	1.58E-03	1.54E-03	1.49E-03
cinnamic acid	6.95E-05	6.95E-05	6.95E-05	6.95E-05	6.95E-05	6.95E-05	6.95E-05	6.94E-05	6.93E-05	6.92E-05	6.90E-05	6.87E-05	6.82E-05	6.74E-05	6.63E-05	6.45E-05	6.19E-05	5.81E-05	5.30E-05	4.65E-05
p-coumaric acid	1.24E-08	1.24E-08	1.24E-08	1.24E-08	1.24E-08	1.24E-08	1.24E-08	1.24E-08	1.24E-08	1.24E-08	1.24E-08	1.23E-08	1.23E-08	1.22E-08	1.21E-08	1.19E-08	1.16E-08	1.11E-08	1.05E-08	9.57E-09
undecylic acid	2.07E-03	2.07E-03	2.07E-03	2.07E-03	2.07E-03	2.07E-03	2.07E-03	2.07E-03	2.07E-03	2.07E-03	2.07E-03	2.06E-03	2.06E-03	2.05E-03	2.05E-03	2.03E-03	2.01E-03	1.98E-03	1.93E-03	1.86E-03
(E)-2-hexenoic acid	2.75E-03	2.75E-03	2.75E-03	2.75E-03	2.75E-03	2.75E-03	2.75E-03	2.75E-03	2.75E-03	2.74E-03	2.74E-03	2.73E-03	2.72E-03	2.70E-03	2.67E-03	2.63E-03	2.56E-03	2.45E-03	2.31E-03	2.10E-03
oleic acid	7.34E-04	7.34E-04	7.34E-04	7.33E-04	7.33E-04	7.33E-04	7.33E-04	7.33E-04	7.33E-04	7.33E-04	7.32E-04	7.31E-04	7.30E-04	7.28E-04	7.25E-04	7.20E-04	7.13E-04	7.02E-04	6.84E-04	6.58E-04
lauric acid	2.54E-03	2.54E-03	2.54E-03	2.54E-03	2.54E-03	2.54E-03	2.54E-03	2.54E-03	2.54E-03	2.54E-03	2.54E-03	2.54E-03	2.53E-03	2.52E-03	2.51E-03	2.50E-03	2.47E-03	2.43E-03	2.37E-03	2.28E-03
phenol	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03
guaiacol	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03
p-cresol	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03
m-cresol	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03
3-ethylphenol	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03
o-cresol	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03
p-vinylguaiacol	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03
4-propyl-guaiacol	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02
syringol	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05
4-vinylphenol	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04

Table S1a. SPARC estimated pH dependent effective air/water partitioning coefficients ($K_{aw,eff}$; atm M^{-1}) for ionizable aroma compounds from the Flavornet database.

pH	4.0	4.2	4.4	4.6	4.8	5.0	5.2	5.4	5.6	5.8	6.0	6.2	6.4	6.6	6.8	7.0	7.2	7.4	7.6	7.8
trimethylamine	1.41E-07	2.24E-07	3.55E-07	5.63E-07	8.93E-07	1.41E-06	2.24E-06	3.55E-06	5.63E-06	8.93E-06	1.41E-05	2.24E-05	3.55E-05	5.63E-05	8.92E-05	1.41E-04	2.24E-04	3.54E-04	5.61E-04	8.86E-04
methanethiol	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.46E+00	2.45E+00	2.45E+00	2.44E+00
pyrrolidine	6.02E-10	9.54E-10	1.51E-09	2.40E-09	3.80E-09	6.02E-09	9.54E-09	1.51E-08	2.40E-08	3.80E-08	6.02E-08	9.54E-08	1.51E-07	2.40E-07	3.80E-07	6.02E-07	9.54E-07	1.51E-06	2.39E-06	3.79E-06
propanoic acid	1.08E-04	9.94E-05	8.80E-05	7.45E-05	5.99E-05	4.57E-05	3.32E-05	2.32E-05	1.57E-05	1.04E-05	6.75E-06	4.34E-06	2.78E-06	1.77E-06	1.12E-06	7.09E-07	4.48E-07	2.83E-07	1.79E-07	1.13E-07
butyric acid	1.97E-04	1.81E-04	1.61E-04	1.36E-04	1.09E-04	8.34E-05	6.06E-05	4.23E-05	2.86E-05	1.89E-05	1.23E-05	7.92E-06	5.06E-06	3.22E-06	2.04E-06	1.29E-06	8.17E-07	5.16E-07	3.26E-07	2.06E-07
acetic acid	6.19E-05	5.71E-05	5.09E-05	4.33E-05	3.51E-05	2.70E-05	1.97E-05	1.38E-05	9.40E-06	6.23E-06	4.06E-06	2.62E-06	1.67E-06	1.06E-06	6.76E-07	4.28E-07	2.70E-07	1.71E-07	1.08E-07	6.81E-08
methylbutenthiol	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.40E-01	7.40E-01
pyridine	1.65E-03	2.45E-03	3.52E-03	4.87E-03	6.41E-03	8.02E-03	9.52E-03	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02
methyl pyrazine	2.74E-03	2.75E-03	2.76E-03	2.76E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03
isovaleric acid	2.98E-04	2.74E-04	2.42E-04	2.05E-04	1.65E-04	1.26E-04	9.16E-05	6.39E-05	4.32E-05	2.86E-05	1.86E-05	1.20E-05	7.64E-06	4.86E-06	3.08E-06	1.95E-06	1.23E-06	7.79E-07	4.92E-07	3.11E-07
methylfuranthiol	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	6.00E-02	6.00E-02	6.00E-02	5.00E-02	4.00E-02	4.00E-02	3.00E-02	2.00E-02	2.00E-02	1.00E-02	6.99E-03	4.58E-03	2.96E-03
methylbutyric acid	5.54E-04	5.06E-04	4.45E-04	3.74E-04	2.99E-04	2.26E-04	1.63E-04	1.13E-04	7.64E-05	5.04E-05	3.27E-05	2.10E-05	1.34E-05	8.53E-06	5.41E-06	3.42E-06	2.16E-06	1.37E-06	8.63E-07	5.45E-07
dimethylthiazole	4.00E-02	4.00E-02	5.00E-02	6.00E-02	6.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02
o-picoline	5.68E-04	8.90E-04	1.38E-03	2.13E-03	3.23E-03	4.78E-03	6.87E-03	9.47E-03	1.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02
methyltetrahydrofuranthiol	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.03E-03	7.02E-03	7.02E-03	7.01E-03	7.00E-03	6.99E-03	6.97E-03	6.93E-03	6.88E-03	6.79E-03
2,5-dimethyl pyrazine	3.81E-03	3.89E-03	3.95E-03	3.99E-03	4.01E-03	4.02E-03	4.03E-03	4.04E-03	4.04E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03
2,6-dimethyl pyrazine	2.13E-03	2.19E-03	2.22E-03	2.25E-03	2.26E-03	2.27E-03	2.28E-03	2.28E-03	2.28E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03
2-ethyl pyrazine	5.13E-03	5.16E-03	5.17E-03	5.18E-03	5.19E-03	5.19E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03
caproic acid	4.00E-04	3.68E-04	3.25E-04	2.75E-04	2.22E-04	1.69E-04	1.23E-04	8.58E-05	5.80E-05	3.84E-05	2.50E-05	1.61E-05	1.03E-05	6.53E-06	4.14E-06	2.62E-06	1.66E-06	1.05E-06	6.61E-07	4.17E-07
pentanoic acid	2.94E-04	2.70E-04	2.39E-04	2.02E-04	1.63E-04	1.24E-04	9.03E-05	6.30E-05	4.26E-05	2.82E-05	1.83E-05	1.18E-05	7.53E-06	4.79E-06	3.04E-06	1.92E-06	1.22E-06	7.68E-07	4.85E-07	3.06E-07
2,3-dimethyl pyrazine	3.13E-03	3.20E-03	3.24E-03	3.27E-03	3.29E-03	3.30E-03	3.31E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03
fufuryl mercaptan	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02
acetylpyrroline	1.43E-07	2.27E-07	3.59E-07	5.69E-07	9.01E-07	1.43E-06	2.25E-06	3.55E-06	5.58E-06	8.74E-06	1.36E-05	2.09E-05	3.17E-05	4.69E-05	6.73E-05	9.28E-05	1.22E-04	1.52E-04	1.80E-04	2.04E-04
methoxymethylbutanethiol	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02	9.00E-02
ethyl mercaptopropionate	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	4.00E-02
4,5-dimethyl thiazole	5.00E-02	6.00E-02	6.00E-02	6.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02
hexanethiol	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.10E+00	6.09E+00	6.09E+00	6.08E+00	6.06E+00
2-methyl-4,5-dihydro-3-furanthiol	9.00E-02	9.00E-02	9.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	7.00E-02	7.00E-02	6.00E-02	5.00E-02	4.00E-02	3.00E-02	2.00E-02	2.00E-02	1.00E-02	7.08E-03	4.61E-03	2.97E-03
4-methyl-3-thiazoline	1.04E-05	1.64E-05	2.60E-05	4.11E-05	6.48E-05	1.02E-04	1.59E-04	2.48E-04	3.81E-04	5.77E-04	8.53E-04	1.22E-03	1.68E-03	2.21E-03	2.75E-03	3.25E-03	3.68E-03	4.01E-03	4.25E-03	4.42E-03
2-ethylpyridine	8.52E-04	1.33E-03	2.07E-03	3.18E-03	4.81E-03	7.11E-03	1.00E-02	1.00E-02	2.00E-02	2.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02
3-mercapto-4-methyl-2-pentanone	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	5.00E-02
3-mercaptothiophene	1.70E-01	1.60E-01	1.50E-01	1.40E-01	1.20E-01	1.00E-01	8.00E-02	6.00E-02	4.00E-02	3.00E-02	2.00E-02	1.00E-02	8.24E-03	5.29E-03	3.37E-03	2.14E-03	1.36E-03	8.59E-04	5.43E-04	3.43E-04
2,5-dimethyl-3-furanthiol	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	4.00E-02	3.00E-02	3.00E-02	2.00E-02	1.00E-02	9.97E-03	6.71E-03	4.42E-03
3-mercapto-3-methyl-1-butanol	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.41E-03
2-ethyl-5-methyl pyrazine	6.59E-03	6.74E-03	6.83E-03	6.89E-03	6.93E-03	6.96E-03	6.97E-03	6.98E-03	6.99E-03	6.99E-03	6.99E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03
2,4,5-trimethylthiazole	1.00E-02	2.00E-02	2.00E-02	3.00E-02	4.00E-02	5.00E-02	6.00E-02	6.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02
2,3,5-trimethylpyrazine	1.76E-03	1.92E-03	2.05E-03	2.13E-03	2.19E-03	2.23E-03	2.25E-03	2.27E-03	2.28E-03	2.29E-03	2.29E-03	2.29E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03
2-acetylpyridine	7.26E-05	7.68E-05	7.97E-05	8.16E-05	8.29E-05	8.37E-05	8.43E-05	8.46E-05	8.48E-05	8.50E-05	8.50E-05	8.51E-05	8.51E-05	8.51E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05
5-methyl-2-furfurylthiol	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02
2-acetylthiazole	6.91E-05	6.97E-05	7.01E-05	7.04E-05	7.06E-05	7.07E-05	7.08E-05	7.08E-05	7.08E-05	7.08E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05
2-propionyl-1-pyrroline	3.09E-07	4.89E-07	7.75E-07	1.23E-06	1.94E-06	3.07E-06	4.85E-06	7.65E-06	1.20E-05	1.88E-05	2.93E-05	4.51E-05	6.83E-05	1.01E-04	1.45E-04	2.00E-04	2.63E-04	3.29E-04	3.90E-04	4.41E-04
2-acetyl-1,4,5,6-tetrahydropyridine	2.63E-04	4.05E-04	6.16E-04	9.18E-04	1.33E-03	1.85E-03	2.46E-03	3.11E-03	3.72E-03	4.26E-03	4.68E-03	4.99E-03	5.21E-03	5.36E-03	5.46E-03	5.53E-03	5.57E-03	5.59E-03	5.61E-03	5.62E-03
2-ethyl-6-methylpyrazine	3.35E-03	3.43E-03	3.49E-03	3.53E-03	3.55E-03	3.56E-03	3.57E-03	3.58E-03	3.58E-03	3.58E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03
2-isobutylthiazole	1.20E-01	1.50E-01	1.70E-01	2.00E-01	2.10E-01	2.20E-01	2.30E-01	2.40E-01	2.40E-01	2.40E-01	2.40E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01
4-mercapto-4-methyl-2-pentanone	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02
2-methyl-3-ethylpyrazine	5.36E-03	5.47E-03	5.55E-03	5.60E-03	5.63E-03	5.65E-03	5.66E-03	5.67E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03
2-methyl-3-thiophenethiol	1.80E-01	1.80E-01	1.80E-01	1.70E-01	1.60E-01	1.50E-01	1.30E-01	1.10E-01	9.00E-02	7.00E-02	5.00E-02	4.00E-02	3.00E-02	2.00E-02	1.00E-02	7.01E-03	4.49E-03	2.86E-03	1.81E-03	1.15E-03
5-isopropyl-2-methylpyrazine	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02
2-methoxy-3,6-dimethylpyrazine	5.48E-05	5.56E-05	5.61E-05	5.64E-05	5.66E-05	5.68E-05	5.69E-05	5.69E-05	5.69E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05
5-ethyl-2,4-dimethylthiazole	2.00E-02	3.00E-02	4.00E-02	6.00E-02	7.00E-02	9.00E-02	1.00E-01	1.10E-01	1.20E-01	1.20E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01
2,5-dimethyl-3-ethylpyrazine	2.60E-03	2.84E-03	3.01E-03	3.14E-03	3.22E-03	3.27E-03	3.31E-03	3.33E-03	3.35E-03	3.35E-03	3.36E-03	3.36E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03
thenylthiol	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.80E-01	1.70E-01
2-ethyl-3,5-dimethylpyrazine	2.92E-03	3.19E-03	3.39E-03	3.53E-03	3.63E-03	3.69E-03	3.73E-03	3.76E-03	3.77E-03	3.78E-03	3.79E-03	3.79E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03
2,3-dimethyl-6-ethylpyrazine	2.63E-03	2.87E-03	3.05E-03	3.18E-03	3.26E-03	3.32E-03	3.35E-03	3.38E-03	3.39E-03	3.40E-03	3.41E-03	3.41E-03	3.41E-03	3.41E-03	3.41E-03	3.41E-03	3.41E-03	3.42E-03	3.42E-03	3.42E-03
2-ethyl-3,5-dimethylpyrazine	2.92E-03	3.19E-03	3.39E-03	3.53E-03	3.63E-03	3.69E-03	3.73E-03	3.76E-03	3.77E-03	3.78E-03	3.79E-03	3.79E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03
2-isopropyl-3-methoxypyrazine	4.77E-04	4.78E-04	4.79E-04	4.80E-04	4.80E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04

2-ethenyl-3,5-dimethylpyrazine	2.34E-03	2.40E-03	2.44E-03	2.47E-03	2.48E-03	2.49E-03	2.50E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03
2-acetyl-2-thiazoline	4.61E-07	7.20E-07	1.11E-06	1.70E-06	2.55E-06	3.71E-06	5.22E-06	7.02E-06	8.97E-06	1.09E-05	1.26E-05	1.39E-05	1.50E-05	1.57E-05	1.62E-05	1.65E-05	1.67E-05	1.69E-05	1.70E-05	1.70E-05
2-acetyl-3,4,5,6-tetrahydropyridine	8.60E-07	1.36E-06	2.16E-06	3.42E-06	5.41E-06	8.56E-06	1.35E-05	2.13E-05	3.35E-05	5.25E-05	8.15E-05	1.25E-04	1.90E-04	2.80E-04	4.02E-04	5.53E-04	7.25E-04	9.01E-04	1.06E-03	1.20E-03
4-mercapto-4-methyl-2-pentanol	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	1.99E-03	1.99E-03	1.99E-03	1.99E-03	1.98E-03	1.98E-03
5-methyl-5(H)-cyclopentapyrazine	8.33E-04	8.53E-04	8.66E-04	8.74E-04	8.80E-04	8.83E-04	8.86E-04	8.87E-04	8.88E-04	8.88E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04
3,5-diethyl-2-methylpyrazine	4.92E-03	5.36E-03	5.69E-03	5.91E-03	6.07E-03	6.17E-03	6.23E-03	6.27E-03	6.30E-03	6.32E-03	6.33E-03	6.33E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03
2,3-diethyl-5-methylpyrazine	5.29E-03	5.77E-03	6.12E-03	6.37E-03	6.53E-03	6.64E-03	6.71E-03	6.76E-03	6.79E-03	6.81E-03	6.82E-03	6.83E-03	6.83E-03	6.83E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03
2-sec-butyl-3-methoxypyrazine	5.77E-04	5.79E-04	5.80E-04	5.80E-04	5.81E-04	5.81E-04	5.81E-04	5.81E-04	5.81E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04
2-phenylethylthiol	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01
2-ethenyl-3-ethyl-5-methylpyrazine	3.48E-03	3.57E-03	3.63E-03	3.67E-03	3.69E-03	3.71E-03	3.72E-03	3.72E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03
2-pentylpyridine	1.70E-03	2.66E-03	4.13E-03	6.34E-03	9.59E-03	1.00E-02	2.00E-02	3.00E-02	4.00E-02	5.00E-02	5.00E-02	6.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	8.00E-02	8.00E-02	8.00E-02
2-isobutyl-3-methoxypyrazine	5.56E-04	5.58E-04	5.59E-04	5.60E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04
isobutyric acid	3.49E-04	3.19E-04	2.81E-04	2.36E-04	1.88E-04	1.43E-04	1.03E-04	7.16E-05	4.82E-05	3.18E-05	2.06E-05	1.33E-05	8.47E-06	5.38E-06	3.41E-06	2.16E-06	1.37E-06	8.63E-07	5.45E-07	3.44E-07
benzothiazole	9.34E-04	9.36E-04	9.38E-04	9.38E-04	9.39E-04	9.39E-04	9.39E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04
3-mercapto-1-hexanol-1-acetate	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02
6,7-dihydro-5-methyl-5H-cyclopentapyrazine	1.64E-03	1.66E-03	1.67E-03	1.68E-03	1.68E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03
phenylacetic acid	6.42E-06	5.55E-06	4.57E-06	3.57E-06	2.65E-06	1.88E-06	1.29E-06	8.62E-07	5.64E-07	3.65E-07	2.34E-07	1.49E-07	9.46E-08	5.99E-08	3.79E-08	2.39E-08	1.51E-08	9.55E-09	6.03E-09	3.80E-09
4-methyl-5-hydroxyethyl-thiazole	1.45E-05	1.56E-05	1.63E-05	1.68E-05	1.72E-05	1.74E-05	1.75E-05	1.76E-05	1.77E-05	1.77E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05
o-aminoacetophenone	5.07E-04	5.10E-04	5.12E-04	5.13E-04	5.14E-04	5.14E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04
nonanoic acid	1.10E-03	1.01E-03	8.92E-04	7.55E-04	6.07E-04	4.63E-04	3.37E-04	2.35E-04	1.59E-04	1.05E-04	6.84E-05	4.40E-05	2.81E-05	1.79E-05	1.13E-05	7.18E-06	4.54E-06	2.87E-06	1.81E-06	1.14E-06
benzoic acid	2.97E-05	2.32E-05	1.72E-05	1.22E-05	8.33E-06	5.55E-06	3.63E-06	2.35E-06	1.50E-06	9.58E-07	6.08E-07	3.85E-07	2.44E-07	1.54E-07	9.72E-08	6.14E-08	3.87E-08	2.44E-08	1.54E-08	9.74E-09
octanoic acid	7.19E-04	6.60E-04	5.85E-04	4.95E-04	3.98E-04	3.04E-04	2.21E-04	1.54E-04	1.04E-04	6.89E-05	4.48E-05	2.88E-05	1.84E-05	1.17E-05	7.43E-06	4.71E-06	2.97E-06	1.88E-06	1.19E-06	7.49E-07
p-menthenethiol	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.20E+00	1.19E+00	1.19E+00	1.19E+00	1.19E+00
methyl quinoxaline	4.29E-04	4.30E-04	4.31E-04	4.31E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04
2-isopentyl-3,6-dimethyl pyrazine	4.69E-03	5.12E-03	5.44E-03	5.66E-03	5.81E-03	5.91E-03	5.97E-03	6.02E-03	6.04E-03	6.06E-03	6.07E-03	6.08E-03	6.08E-03	6.08E-03	6.08E-03	6.08E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03
hydrocinnamic acid	8.30E-06	7.42E-06	6.36E-06	5.18E-06	4.00E-06	2.94E-06	2.07E-06	1.41E-06	9.39E-07	6.13E-07	3.95E-07	2.53E-07	1.61E-07	1.02E-07	6.47E-08	4.09E-08	2.59E-08	1.63E-08	1.03E-08	6.51E-09
4-methylthiazole	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02
methyl anthranilate	3.89E-04	3.90E-04	3.91E-04	3.92E-04	3.92E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04
decanoic acid	1.40E-03	1.29E-03	1.14E-03	9.65E-04	7.76E-04	5.92E-04	4.31E-04	3.01E-04	2.03E-04	1.34E-04	8.74E-05	5.63E-05	3.59E-05	2.29E-05	1.45E-05	9.18E-06	5.80E-06	3.67E-06	2.32E-06	1.46E-06
cinnamic acid	3.90E-05	3.10E-05	2.34E-05	1.69E-05	1.17E-05	7.86E-06	5.18E-06	3.36E-06	2.16E-06	1.38E-06	8.75E-07	5.55E-07	3.51E-07	2.22E-07	1.40E-07	8.85E-08	5.59E-08	3.53E-08	2.23E-08	1.40E-08
p-coumaric acid	8.45E-09	7.12E-09	5.70E-09	4.33E-09	3.13E-09	2.18E-09	1.47E-09	9.70E-10	6.30E-10	4.05E-10	2.59E-10	1.64E-10	1.04E-10	6.57E-11	4.14E-11	2.60E-11	1.63E-11	1.01E-11	6.27E-12	3.83E-12
undecylic acid	1.75E-03	1.61E-03	1.43E-03	1.21E-03	9.71E-04	7.41E-04	5.39E-04	3.76E-04	2.54E-04	1.68E-04	1.09E-04	7.04E-05	4.50E-05	2.86E-05	1.81E-05	1.15E-05	7.26E-06	4.59E-06	2.90E-06	1.83E-06
(E)-2-hexenoic acid	1.85E-03	1.55E-03	1.24E-03	9.35E-04	6.74E-04	4.68E-04	3.15E-04	2.07E-04	1.35E-04	8.65E-05	5.52E-05	3.51E-05	2.23E-05	1.41E-05	8.90E-06	5.62E-06	3.55E-06	2.24E-06	1.41E-06	8.93E-07
oleic acid	6.21E-04	5.70E-04	5.04E-04	4.26E-04	3.42E-04	2.61E-04	1.90E-04	1.32E-04	8.94E-05	5.91E-05	3.84E-05	2.47E-05	1.58E-05	1.00E-05	6.37E-06	4.03E-06	2.55E-06	1.61E-06	1.02E-06	6.42E-07
lauric acid	2.16E-03	1.98E-03	1.75E-03	1.48E-03	1.19E-03	9.11E-04	6.62E-04	4.62E-04	3.13E-04	2.07E-04	1.34E-04	8.65E-05	5.53E-05	3.52E-05	2.23E-05	1.41E-05	8.92E-06	5.64E-06	3.56E-06	2.25E-06
phenol	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.61E-03	1.60E-03	1.60E-03	1.60E-03
guaiacol	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.55E-03	5.54E-03	5.54E-03	5.54E-03	5.53E-03	5.53E-03	5.52E-03	5.50E-03
p-cresol	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.74E-03	1.73E-03	1.73E-03	1.73E-03
m-cresol	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.91E-03	1.90E-03	1.90E-03	1.90E-03
3-ethylphenol	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.23E-03	2.22E-03
o-cresol	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.40E-03	1.39E-03	1.39E-03	1.39E-03
p-vinylguaiacol	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.35E-03	2.34E-03	2.34E-03	2.33E-03	2.32E-03	2.31E-03	2.29E-03
4-propyl-guaiacol	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02
syringol	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.60E-05	2.60E-05	2.60E-05	2.60E-05	2.60E-05	2.59E-05	2.58E-05	2.57E-05	2.55E-05	2.51E-05
4-vinylphenol	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.75E-04	6.74E-04	6.74E-04	6.73E-04	6.71E-04	6.69E-04	6.65E-04	6.59E-04

Table S1a. SPARC estimated pH dependent effective air/water partitioning coefficients ($K_{aw,eff}$; atm M^{-1}) for ionizable aroma compounds from the Flavornet database.

pH	8.0	8.2	8.4	8.6	8.8	9.0	9.2	9.4	9.6	9.8	10.0	10.2	10.4	10.6	10.8	11.0	11.2	11.4	11.6	11.8
trimethylamine	1.40E-03	2.20E-03	3.46E-03	5.39E-03	8.34E-03	1.00E-02	2.00E-02	3.00E-02	4.00E-02	5.00E-02	7.00E-02	8.00E-02	9.00E-02	1.00E-01	1.10E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01
methanethiol	2.43E+00	2.41E+00	2.39E+00	2.34E+00	2.28E+00	2.19E+00	2.05E+00	1.87E+00	1.64E+00	1.37E+00	1.09E+00	8.20E-01	5.90E-01	4.10E-01	2.70E-01	1.80E-01	1.20E-01	8.00E-02	5.00E-02	3.00E-02
pyrrolidine	6.01E-06	9.52E-06	1.51E-05	2.39E-05	3.77E-05	5.95E-05	9.38E-05	1.47E-04	2.30E-04	3.55E-04	5.43E-04	8.15E-04	1.19E-03	1.68E-03	2.26E-03	2.90E-03	3.52E-03	4.08E-03	4.53E-03	4.87E-03
propanoic acid	7.12E-08	4.49E-08	2.84E-08	1.79E-08	1.13E-08	7.13E-09	4.50E-09	2.84E-09	1.79E-09	1.13E-09	7.13E-10	4.50E-10	2.84E-10	1.79E-10	1.13E-10	7.13E-11	4.50E-11	2.84E-11	1.79E-11	1.13E-11
butyric acid	1.30E-07	8.20E-08	5.17E-08	3.26E-08	2.06E-08	1.30E-08	8.20E-09	5.17E-09	3.26E-09	2.06E-09	1.30E-09	8.20E-10	5.17E-10	3.26E-10	2.06E-10	1.30E-10	8.20E-11	5.17E-11	3.26E-11	2.06E-11
acetic acid	4.30E-08	2.71E-08	1.71E-08	1.08E-08	6.82E-09	4.30E-09	2.71E-09	1.71E-09	1.08E-09	6.82E-10	4.30E-10	2.71E-10	1.71E-10	1.08E-10	6.82E-11	4.30E-11	2.71E-11	1.71E-11	1.08E-11	6.82E-12
methylbutenthiol	7.40E-01	7.30E-01	7.20E-01	7.10E-01	6.90E-01	6.60E-01	6.20E-01	5.60E-01	4.90E-01	4.00E-01	3.20E-01	2.40E-01	1.70E-01	1.20E-01	8.00E-02	5.00E-02	3.00E-02	2.00E-02	1.00E-02	8.61E-03
pyridine	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02
methyl pyrazine	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03
isovaleric acid	1.96E-07	1.24E-07	7.81E-08	4.93E-08	3.11E-08	1.96E-08	1.24E-08	7.81E-09	4.93E-09	3.11E-09	1.96E-09	1.24E-09	7.81E-10	4.93E-10	3.11E-10	1.96E-10	1.24E-10	7.81E-11	4.93E-11	3.11E-11
methylfuranthiol	1.90E-03	1.21E-03	7.69E-04	4.87E-04	3.08E-04	1.95E-04	1.23E-04	7.77E-05	4.90E-05	3.09E-05	1.95E-05	1.23E-05	7.78E-06	4.91E-06	3.10E-06	1.95E-06	1.23E-06	7.78E-07	4.91E-07	3.10E-07
methylbutyric acid	3.44E-07	2.17E-07	1.37E-07	8.64E-08	5.45E-08	3.44E-08	2.17E-08	1.37E-08	8.64E-09	5.45E-09	3.44E-09	2.17E-09	1.37E-09	8.64E-10	5.45E-10	3.44E-10	2.17E-10	1.37E-10	8.64E-11	5.45E-11
dimethylthiazole	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02
o-picoline	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02
methyltetrahydrofuranthiol	6.65E-03	6.45E-03	6.16E-03	5.74E-03	5.18E-03	4.49E-03	3.71E-03	2.90E-03	2.16E-03	1.54E-03	1.06E-03	7.06E-04	4.62E-04	2.99E-04	1.92E-04	1.22E-04	7.76E-05	4.92E-05	3.11E-05	1.97E-05
2,5-dimethyl pyrazine	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03
2,6-dimethyl pyrazine	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03
2-ethyl pyrazine	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03
caproic acid	2.63E-07	1.66E-07	1.05E-07	6.62E-08	4.17E-08	2.63E-08	1.66E-08	1.05E-08	6.62E-09	4.18E-09	2.63E-09	1.66E-09	1.05E-09	6.62E-10	4.18E-10	2.63E-10	1.66E-10	1.05E-10	6.62E-11	4.18E-11
pentanoic acid	1.93E-07	1.22E-07	7.70E-08	4.86E-08	3.07E-08	1.93E-08	1.22E-08	7.70E-09	4.86E-09	3.07E-09	1.93E-09	1.22E-09	7.70E-10	4.86E-10	3.07E-10	1.93E-10	1.22E-10	7.70E-11	4.86E-11	3.07E-11
2,3-dimethyl pyrazine	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03
fufuryl mercaptan	6.00E-02	6.00E-02	6.00E-02	5.00E-02	5.00E-02	4.00E-02	3.00E-02	2.00E-02	2.00E-02	1.00E-02	7.40E-03	4.86E-03	3.15E-03	2.02E-03	1.29E-03	8.19E-04	5.19E-04	3.28E-04	2.07E-04	1.31E-04
acetylpyrroline	2.23E-04	2.36E-04	2.46E-04	2.52E-04	2.56E-04	2.59E-04	2.61E-04	2.62E-04	2.62E-04	2.63E-04	2.63E-04	2.63E-04	2.63E-04	2.63E-04	2.63E-04	2.63E-04	2.63E-04	2.64E-04	2.64E-04	2.64E-04
methoxymethylbutanethiol	9.00E-02	9.00E-02	8.00E-02	8.00E-02	8.00E-02	7.00E-02	7.00E-02	6.00E-02	5.00E-02	4.00E-02	3.00E-02	2.00E-02	2.00E-02	1.00E-02	7.07E-03	4.60E-03	2.96E-03	1.89E-03	1.20E-03	7.62E-04
ethyl mercaptopropionate	4.00E-02	4.00E-02	3.00E-02	2.00E-02	2.00E-02	1.00E-02	8.35E-03	5.58E-03	3.66E-03	2.37E-03	1.52E-03	9.68E-04	6.15E-04	3.89E-04	2.46E-04	1.56E-04	9.83E-05	6.21E-05	3.92E-05	2.47E-05
4,5-dimethyl thiazole	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02
hexanethiol	6.04E+00	6.00E+00	5.94E+00	5.84E+00	5.70E+00	5.49E+00	5.18E+00	4.76E+00	4.22E+00	3.57E+00	2.87E+00	2.20E+00	1.60E+00	1.12E+00	7.50E-01	5.00E-01	3.20E-01	2.10E-01	1.30E-01	8.00E-02
2-methyl-4,5-dihydro-3-furanthiol	1.90E-03	1.21E-03	7.65E-04	4.84E-04	3.06E-04	1.93E-04	1.22E-04	7.71E-05	4.86E-05	3.07E-05	1.94E-05	1.22E-05	7.71E-06	4.87E-06	3.07E-06	1.94E-06	1.22E-06	7.71E-07	4.87E-07	3.07E-07
4-methyl-3-thiazoline	4.53E-03	4.60E-03	4.65E-03	4.68E-03	4.70E-03	4.71E-03	4.72E-03	4.73E-03	4.73E-03	4.73E-03	4.73E-03	4.73E-03	4.73E-03	4.73E-03	4.74E-03	4.74E-03	4.74E-03	4.74E-03	4.74E-03	4.74E-03
2-ethylpyridine	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02
3-mercapto-4-methyl-2-pentanone	5.00E-02	5.00E-02	5.00E-02	4.00E-02	4.00E-02	3.00E-02	2.00E-02	2.00E-02	1.00E-02	9.15E-03	6.13E-03	4.03E-03	2.61E-03	1.67E-03	1.07E-03	6.78E-04	4.29E-04	2.72E-04	1.72E-04	1.08E-04
3-mercaptothiophene	2.17E-04	1.37E-04	8.63E-05	5.45E-05	3.44E-05	2.17E-05	1.37E-05	8.63E-06	5.45E-06	3.44E-06	2.17E-06	1.37E-06	8.63E-07	5.45E-07	3.44E-07	2.17E-07	1.37E-07	8.63E-08	5.45E-08	3.44E-08
2,5-dimethyl-3-furanthiol	2.87E-03	1.84E-03	1.17E-03	7.47E-04	4.73E-04	3.00E-04	1.89E-04	1.20E-04	7.55E-05	4.77E-05	3.01E-05	1.90E-05	1.20E-05	7.56E-06	4.77E-06	3.01E-06	1.90E-06	1.20E-06	7.56E-07	4.77E-07
3-mercapto-3-methyl-1-butanol	1.40E-03	1.39E-03	1.38E-03	1.35E-03	1.31E-03	1.25E-03	1.16E-03	1.05E-03	9.07E-04	7.48E-04	5.85E-04	4.35E-04	3.09E-04	2.12E-04	1.42E-04	9.28E-05	6.00E-05	3.84E-05	2.45E-05	1.56E-05
2-ethyl-5-methyl pyrazine	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03
2,4,5-trimethylthiazole	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02
2,3,5-trimethylpyrazine	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03
2-acetylpyridine	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05
5-methyl-2-furfurylthiol	5.00E-02	5.00E-02	5.00E-02	4.00E-02	4.00E-02	3.00E-02	3.00E-02	2.00E-02	2.00E-02	1.00E-02	8.45E-03	5.67E-03	3.73E-03	2.42E-03	1.55E-03	9.90E-04	6.29E-04	3.99E-04	2.52E-04	1.59E-04
2-acetylthiazole	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05
2-propionyl-1-pyrroline	4.81E-04	5.11E-04	5.31E-04	5.45E-04	5.54E-04	5.60E-04	5.64E-04	5.66E-04	5.68E-04	5.69E-04	5.69E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04
2-acetyl-1,4,5,6-tetrahydropyridine	5.63E-03	5.63E-03	5.63E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03
2-ethyl-6-methylpyrazine	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03
2-isobutylthiazole	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01
4-mercapto-4-methyl-2-pentanone	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	1.00E-02	1.00E-02	1.00E-02	9.24E-03	7.13E-03	5.23E-03	3.68E-03	2.50E-03	1.66E-03	1.08E-03	6.99E-04	4.47E-04	2.85E-04
2-methyl-3-ethylpyrazine	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03
2-methyl-3-thiophenethiol	7.25E-04	4.58E-04	2.89E-04	1.83E-04	1.15E-04	7.28E-05	4.59E-05	2.90E-05	1.83E-05	1.15E-05	7.28E-06	4.60E-06	2.90E-06	1.83E-06	1.15E-06	7.28E-07	4.60E-07	2.90E-07	1.83E-07	1.15E-07
5-isopropyl-2-methylpyrazine	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02
2-methoxy-3,6-dimethylpyrazine	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05
5-ethyl-2,4-dimethylthiazole	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01
2,5-dimethyl-3-ethylpyrazine	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03
thenylthiol	1.70E-01	1.60E-01	1.50E-01	1.30E-01	1.10E-01	9.00E-02	7.00E-02	5.00E-02	3.00E-02	2.00E-02	2.00E-02	1.00E-02	6.55E-03	4.19E-03	2.66E-03	1.69E-03	1.07E-03	6.77E-04	4.27E-04	2.70E-04
2-ethyl-3,5-dimethylpyrazine	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03
2,3-dimethyl-6-ethylpyrazine	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03
2-ethyl-3,5-dimethylpyrazine	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03
2-isopropyl-3-methoxypyrazine	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04

2-ethenyl-3,5-dimethylpyrazine	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03
2-acetyl-2-thiazoline	1.70E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05
2-acetyl-3,4,5,6-tetrahydropyridine	1.31E-03	1.39E-03	1.44E-03	1.48E-03	1.50E-03	1.52E-03	1.53E-03	1.53E-03	1.54E-03	1.54E-03	1.54E-03	1.54E-03	1.54E-03	1.54E-03	1.54E-03	1.54E-03	1.54E-03	1.55E-03	1.55E-03	1.55E-03
4-mercapto-4-methyl-2-pentanol	1.97E-03	1.95E-03	1.93E-03	1.89E-03	1.83E-03	1.75E-03	1.63E-03	1.47E-03	1.27E-03	1.05E-03	8.20E-04	6.09E-04	4.33E-04	2.97E-04	1.98E-04	1.30E-04	8.40E-05	5.39E-05	3.43E-05	2.18E-05
5-methyl-5(H)-cyclopentapyrazine	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04
3,5-diethyl-2-methylpyrazine	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03
2,3-diethyl-5-methylpyrazine	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03
2-sec-butyl-3-methoxypyrazine	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04
2-phenylethylthiol	1.20E-01	1.10E-01	1.10E-01	1.10E-01	1.10E-01	1.00E-01	9.00E-02	8.00E-02	7.00E-02	5.00E-02	4.00E-02	3.00E-02	2.00E-02	1.00E-02	9.18E-03	5.97E-03	3.84E-03	2.45E-03	1.56E-03	9.88E-04
2-ethenyl-3-ethyl-5-methylpyrazine	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03
2-pentylpyridine	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02
2-isobutyl-3-methoxypyrazine	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04
isobutyric acid	2.17E-07	1.37E-07	8.64E-08	5.45E-08	3.44E-08	2.17E-08	1.37E-08	8.64E-09	5.45E-09	3.44E-09	2.17E-09	1.37E-09	8.64E-10	5.45E-10	3.44E-10	2.17E-10	1.37E-10	8.64E-11	5.45E-11	3.44E-11
benzothiazole	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04
3-mercapto-1-hexanol-1-acetate	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	1.00E-02	1.00E-02	9.25E-03	6.94E-03	4.98E-03	3.44E-03	2.30E-03	1.51E-03	9.81E-04	6.30E-04	4.02E-04	2.55E-04	1.62E-04	1.02E-04
6,7-dihydro-5-methyl-5H-cyclopentapyrazine	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03
phenylacetic acid	2.40E-09	1.51E-09	9.56E-10	6.03E-10	3.81E-10	2.40E-10	1.52E-10	9.56E-11	6.03E-11	3.81E-11	2.40E-11	1.52E-11	9.56E-12	6.03E-12	3.81E-12	2.40E-12	1.52E-12	9.56E-13	6.03E-13	3.81E-13
4-methyl-5-hydroxyethyl-thiazole	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05
o-aminoacetophenone	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04
nonanoic acid	7.22E-07	4.56E-07	2.87E-07	1.81E-07	1.14E-07	7.22E-08	4.56E-08	2.88E-08	1.81E-08	1.14E-08	7.22E-09	4.56E-09	2.88E-09	1.81E-09	1.14E-09	7.22E-10	4.56E-10	2.88E-10	1.81E-10	1.14E-10
benzoic acid	6.14E-09	3.88E-09	2.45E-09	1.54E-09	9.74E-10	6.14E-10	3.88E-10	2.45E-10	1.54E-10	9.74E-11	6.14E-11	3.88E-11	2.45E-11	1.54E-11	9.74E-12	6.14E-12	3.88E-12	2.45E-12	1.54E-12	9.74E-13
octanoic acid	4.73E-07	2.98E-07	1.88E-07	1.19E-07	7.50E-08	4.73E-08	2.99E-08	1.88E-08	1.19E-08	7.50E-09	4.73E-09	2.99E-09	1.88E-09	1.19E-09	7.50E-10	4.73E-10	2.99E-10	1.88E-10	1.19E-10	7.50E-11
p-menthenethiol	1.19E+00	1.18E+00	1.18E+00	1.16E+00	1.15E+00	1.12E+00	1.08E+00	1.02E+00	9.40E-01	8.40E-01	7.20E-01	5.80E-01	4.50E-01	3.30E-01	2.30E-01	1.60E-01	1.00E-01	7.00E-02	4.00E-02	3.00E-02
methyl quinoxaline	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04
2-isopentyl-3,6-dimethyl pyrazine	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03
hydrocinnamic acid	4.11E-09	2.59E-09	1.64E-09	1.03E-09	6.51E-10	4.11E-10	2.59E-10	1.64E-10	1.03E-10	6.51E-11	4.11E-11	2.59E-11	1.64E-11	1.03E-11	6.51E-12	4.11E-12	2.59E-12	1.64E-12	1.03E-12	6.51E-13
4-methylthiazole	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02
methyl anthranilate	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04
decanoic acid	9.22E-07	5.82E-07	3.67E-07	2.32E-07	1.46E-07	9.23E-08	5.82E-08	3.67E-08	2.32E-08	1.46E-08	9.23E-09	5.82E-09	3.67E-09	2.32E-09	1.46E-09	9.23E-10	5.82E-10	3.67E-10	2.32E-10	1.46E-10
cinnamic acid	8.86E-09	5.59E-09	3.53E-09	2.23E-09	1.41E-09	8.87E-10	5.59E-10	3.53E-10	2.23E-10	1.41E-10	8.87E-11	5.59E-11	3.53E-11	2.23E-11	1.41E-11	8.87E-12	5.59E-12	3.53E-12	2.23E-12	1.41E-12
p-coumaric acid	2.30E-12	1.35E-12	7.67E-13	4.18E-13	2.16E-13	1.06E-13	4.98E-14	2.23E-14	9.62E-15	4.05E-15	1.67E-15	6.81E-16	2.75E-16	1.11E-16	4.43E-17	1.77E-17	7.07E-18	2.82E-18	1.12E-18	4.47E-19
undecylic acid	1.15E-06	7.29E-07	4.60E-07	2.90E-07	1.83E-07	1.15E-07	7.29E-08	4.60E-08	2.90E-08	1.83E-08	1.16E-08	7.29E-09	4.60E-09	2.90E-09	1.83E-09	1.16E-09	7.29E-10	4.60E-10	2.90E-10	1.83E-10
(E)-2-hexenoic acid	5.63E-07	3.56E-07	2.24E-07	1.42E-07	8.93E-08	5.64E-08	3.56E-08	2.24E-08	1.42E-08	8.93E-09	5.64E-09	3.56E-09	2.24E-09	1.42E-09	8.93E-10	5.64E-10	3.56E-10	2.24E-10	1.42E-10	8.93E-11
oleic acid	4.05E-07	2.56E-07	1.61E-07	1.02E-07	6.42E-08	4.05E-08	2.56E-08	1.61E-08	1.02E-08	6.42E-09	4.05E-09	2.56E-09	1.61E-09	1.02E-09	6.42E-10	4.05E-10	2.56E-10	1.61E-10	1.02E-10	6.42E-11
lauric acid	1.42E-06	8.95E-07	5.65E-07	3.56E-07	2.25E-07	1.42E-07	8.96E-08	5.65E-08	3.57E-08	2.25E-08	1.42E-08	8.96E-09	5.65E-09	3.57E-09	2.25E-09	1.42E-09	8.96E-10	5.65E-10	3.57E-10	2.25E-10
phenol	1.59E-03	1.58E-03	1.56E-03	1.53E-03	1.49E-03	1.43E-03	1.35E-03	1.23E-03	1.08E-03	9.08E-04	7.24E-04	5.48E-04	3.95E-04	2.74E-04	1.85E-04	1.22E-04	7.90E-05	5.07E-05	3.24E-05	2.06E-05
guaiacol	5.47E-03	5.43E-03	5.36E-03	5.25E-03	5.10E-03	4.87E-03	4.54E-03	4.10E-03	3.56E-03	2.95E-03	2.31E-03	1.72E-03	1.23E-03	8.44E-04	5.64E-04	3.70E-04	2.39E-04	1.53E-04	9.77E-05	6.21E-05
p-cresol	1.73E-03	1.72E-03	1.71E-03	1.70E-03	1.68E-03	1.64E-03	1.60E-03	1.52E-03	1.42E-03	1.28E-03	1.12E-03	9.22E-04	7.24E-04	5.40E-04	3.85E-04	2.64E-04	1.77E-04	1.16E-04	7.49E-05	4.80E-05
m-cresol	1.89E-03	1.88E-03	1.87E-03	1.84E-03	1.81E-03	1.76E-03	1.68E-03	1.57E-03	1.42E-03	1.24E-03	1.03E-03	8.07E-04	6.03E-04	4.31E-04	2.97E-04	1.98E-04	1.30E-04	8.43E-05	5.41E-05	3.45E-05
3-ethylphenol	2.21E-03	2.20E-03	2.19E-03	2.16E-03	2.12E-03	2.06E-03	1.97E-03	1.84E-03	1.66E-03	1.45E-03	1.20E-03	9.44E-04	7.06E-04	5.04E-04	3.47E-04	2.32E-04	1.52E-04	9.87E-05	6.33E-05	4.04E-05
o-cresol	1.39E-03	1.39E-03	1.38E-03	1.37E-03	1.36E-03	1.33E-03	1.30E-03	1.25E-03	1.17E-03	1.07E-03	9.43E-04	7.93E-04	6.33E-04	4.79E-04	3.46E-04	2.41E-04	1.62E-04	1.07E-04	6.94E-05	4.46E-05
p-vinylguaiacol	2.25E-03	2.20E-03	2.11E-03	2.00E-03	1.84E-03	1.63E-03	1.38E-03	1.11E-03	8.51E-04	6.20E-04	4.33E-04	2.93E-04	1.94E-04	1.26E-04	8.13E-05	5.20E-05	3.31E-05	2.10E-05	1.33E-05	8.39E-06
4-propyl-guaiacol	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	9.98E-03	9.65E-03	9.15E-03	8.47E-03	7.57E-03	6.48E-03	5.28E-03	4.08E-03	3.00E-03	2.11E-03	1.44E-03	9.55E-04	6.23E-04	4.02E-04	2.57E-04
syringol	2.46E-05	2.39E-05	2.27E-05	2.11E-05	1.90E-05	1.65E-05	1.35E-05	1.06E-05	7.84E-06	5.56E-06	3.81E-06	2.54E-06	1.66E-06	1.07E-06	6.89E-07	4.39E-07	2.79E-07	1.76E-07	1.12E-07	7.06E-08
4-vinylphenol	6.49E-04	6.35E-04	6.14E-04	5.83E-04	5.39E-04	4.82E-04	4.13E-04	3.37E-04	2.60E-04	1.92E-04	1.35E-04	9.20E-05	6.11E-05	3.99E-05	2.57E-05	1.65E-05	1.05E-05	6.65E-06	4.21E-06	2.66E-06

Table S1a. SPARC estimated pH dependent effective air/water partitioning coefficients ($K_{aw,eff}$; atm M^{-1}) for ionizable aroma compounds from the Flavornet database.

pH	12.0	12.2	12.4	12.6	12.8	13.0	13.2	13.4	13.6	13.8	14.0
trimethylamine	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01
methanethiol	2.00E-02	1.00E-02	7.74E-03	4.89E-03	3.09E-03	1.95E-03	1.23E-03	7.77E-04	4.90E-04	3.09E-04	1.95E-04
pyrrolidine	5.11E-03	5.28E-03	5.38E-03	5.46E-03	5.50E-03	5.53E-03	5.55E-03	5.56E-03	5.57E-03	5.58E-03	5.58E-03
propanoic acid	7.13E-12	4.50E-12	2.84E-12	1.79E-12	1.13E-12	7.13E-13	4.50E-13	2.84E-13	1.79E-13	1.13E-13	7.13E-14
butyric acid	1.30E-11	8.20E-12	5.17E-12	3.26E-12	2.06E-12	1.30E-12	8.20E-13	5.17E-13	3.26E-13	2.06E-13	1.30E-13
acetic acid	4.30E-12	2.71E-12	1.71E-12	1.08E-12	6.82E-13	4.30E-13	2.71E-13	1.71E-13	1.08E-13	6.82E-14	4.30E-14
methylbutenthiol	5.46E-03	3.45E-03	2.18E-03	1.38E-03	8.70E-04	5.49E-04	3.47E-04	2.19E-04	1.38E-04	8.71E-05	5.50E-05
pyridine	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02
methyl pyrazine	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03	2.77E-03
isovaleric acid	1.96E-11	1.24E-11	7.81E-12	4.93E-12	3.11E-12	1.96E-12	1.24E-12	7.81E-13	4.93E-13	3.11E-13	1.96E-13
methylfuranthiol	1.95E-07	1.23E-07	7.78E-08	4.91E-08	3.10E-08	1.95E-08	1.23E-08	7.78E-09	4.91E-09	3.10E-09	1.95E-09
methylbutyric acid	3.44E-11	2.17E-11	1.37E-11	8.64E-12	5.45E-12	3.44E-12	2.17E-12	1.37E-12	8.64E-13	5.45E-13	3.44E-13
dimethylthiazole	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02
o-picoline	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02
methyltetrahydrofuranthiol	1.24E-05	7.84E-06	4.95E-06	3.12E-06	1.97E-06	1.24E-06	7.85E-07	4.95E-07	3.12E-07	1.97E-07	1.24E-07
2,5-dimethyl pyrazine	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03	4.05E-03
2,6-dimethyl pyrazine	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03	2.29E-03
2-ethyl pyrazine	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03	5.20E-03
caproic acid	2.63E-11	1.66E-11	1.05E-11	6.62E-12	4.18E-12	2.63E-12	1.66E-12	1.05E-12	6.62E-13	4.18E-13	2.63E-13
pentanoic acid	1.93E-11	1.22E-11	7.70E-12	4.86E-12	3.07E-12	1.93E-12	1.22E-12	7.70E-13	4.86E-13	3.07E-13	1.93E-13
2,3-dimethyl pyrazine	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03	3.32E-03
fufuryl mercaptan	8.27E-05	5.22E-05	3.30E-05	2.08E-05	1.31E-05	8.28E-06	5.23E-06	3.30E-06	2.08E-06	1.31E-06	8.28E-07
acetylpyrroline	2.64E-04	2.64E-04	2.64E-04	2.64E-04	2.64E-04	2.64E-04	2.64E-04	2.64E-04	2.64E-04	2.64E-04	2.64E-04
methoxymethylbutanethiol	4.82E-04	3.05E-04	1.93E-04	1.22E-04	7.68E-05	4.85E-05	3.06E-05	1.93E-05	1.22E-05	7.68E-06	4.85E-06
ethyl mercaptopropionate	1.56E-05	9.85E-06	6.21E-06	3.92E-06	2.47E-06	1.56E-06	9.85E-07	6.21E-07	3.92E-07	2.47E-07	1.56E-07
4,5-dimethyl thiazole	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02	7.00E-02
hexanethiol	5.00E-02	3.00E-02	2.00E-02	1.00E-02	8.60E-03	5.43E-03	3.43E-03	2.16E-03	1.36E-03	8.61E-04	5.43E-04
2-methyl-4,5-dihydro-3-furanthiol	1.94E-07	1.22E-07	7.71E-08	4.87E-08	3.07E-08	1.94E-08	1.22E-08	7.71E-09	4.87E-09	3.07E-09	1.94E-09
4-methyl-3-thiazoline	4.74E-03	4.74E-03	4.74E-03	4.74E-03	4.74E-03	4.74E-03	4.74E-03	4.74E-03	4.74E-03	4.74E-03	4.74E-03
2-ethylpyridine	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02
3-mercapto-4-methyl-2-pentanone	6.85E-05	4.32E-05	2.73E-05	1.72E-05	1.09E-05	6.86E-06	4.33E-06	2.73E-06	1.72E-06	1.09E-06	6.86E-07
3-mercaptothiophene	2.17E-08	1.37E-08	8.63E-09	5.45E-09	3.44E-09	2.17E-09	1.37E-09	8.63E-10	5.45E-10	3.44E-10	2.17E-10
2,5-dimethyl-3-furanthiol	3.01E-07	1.90E-07	1.20E-07	7.56E-08	4.77E-08	3.01E-08	1.90E-08	1.20E-08	7.56E-09	4.77E-09	3.01E-09
3-mercapto-3-methyl-1-butanol	9.85E-06	6.23E-06	3.94E-06	2.49E-06	1.57E-06	9.92E-07	6.26E-07	3.95E-07	2.49E-07	1.57E-07	9.92E-08
2-ethyl-5-methyl pyrazine	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03	7.00E-03
2,4,5-trimethylthiazole	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02
2,3,5-trimethylpyrazine	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03	2.30E-03
2-acetylpyridine	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05	8.52E-05
5-methyl-2-furfurylthiol	1.01E-04	6.36E-05	4.02E-05	2.53E-05	1.60E-05	1.01E-05	6.37E-06	4.02E-06	2.54E-06	1.60E-06	1.01E-06
2-acetylthiazole	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05	7.09E-05
2-propionyl-1-pyrroline	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04	5.70E-04
2-acetyl-1,4,5,6-tetrahydropyridine	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03	5.64E-03
2-ethyl-6-methylpyrazine	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03	3.59E-03
2-isobutylthiazole	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01	2.50E-01
4-mercapto-4-methyl-2-pentanone	1.81E-04	1.14E-04	7.23E-05	4.57E-05	2.89E-05	1.82E-05	1.15E-05	7.26E-06	4.58E-06	2.89E-06	1.82E-06
2-methyl-3-ethylpyrazine	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03	5.68E-03
2-methyl-3-thiophenethiol	7.28E-08	4.60E-08	2.90E-08	1.83E-08	1.15E-08	7.28E-09	4.60E-09	2.90E-09	1.83E-09	1.15E-09	7.28E-10
5-isopropyl-2-methylpyrazine	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02
2-methoxy-3,6-dimethylpyrazine	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05	5.70E-05
5-ethyl-2,4-dimethylthiazole	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01	1.30E-01
2,5-dimethyl-3-ethylpyrazine	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03	3.37E-03
thenylthiol	1.70E-04	1.08E-04	6.79E-05	4.28E-05	2.70E-05	1.71E-05	1.08E-05	6.79E-06	4.28E-06	2.70E-06	1.71E-06
2-ethyl-3,5-dimethylpyrazine	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03
2,3-dimethyl-6-ethylpyrazine	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03	3.42E-03
2-ethyl-3,5-dimethylpyrazine	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03	3.80E-03
2-isopropyl-3-methoxypyrazine	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04	4.81E-04

2-ethenyl-3,5-dimethylpyrazine	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03	2.51E-03
2-acetyl-2-thiazoline	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05	1.71E-05
2-acetyl-3,4,5,6-tetrahydropyridine	1.55E-03	1.55E-03	1.55E-03	1.55E-03	1.55E-03	1.55E-03	1.55E-03	1.55E-03	1.55E-03	1.55E-03	1.55E-03
4-mercapto-4-methyl-2-pentanol	1.38E-05	8.73E-06	5.52E-06	3.49E-06	2.20E-06	1.39E-06	8.77E-07	5.53E-07	3.49E-07	2.20E-07	1.39E-07
5-methyl-5(H)-cyclopentapyrazine	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04	8.89E-04
3,5-diethyl-2-methylpyrazine	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03	6.34E-03
2,3-diethyl-5-methylpyrazine	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03	6.84E-03
2-sec-butyl-3-methoxypyrazine	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04	5.82E-04
2-phenylethylthiol	6.25E-04	3.95E-04	2.50E-04	1.58E-04	9.95E-05	6.28E-05	3.96E-05	2.50E-05	1.58E-05	9.96E-06	6.29E-06
2-ethenyl-3-ethyl-5-methylpyrazine	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03	3.73E-03
2-pentylpyridine	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02	8.00E-02
2-isobutyl-3-methoxypyrazine	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04	5.61E-04
isobutyric acid	2.17E-11	1.37E-11	8.64E-12	5.45E-12	3.44E-12	2.17E-12	1.37E-12	8.64E-13	5.45E-13	3.44E-13	2.17E-13
benzothiazole	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04	9.40E-04
3-mercapto-1-hexanol-1-acetate	6.47E-05	4.08E-05	2.58E-05	1.63E-05	1.03E-05	6.48E-06	4.09E-06	2.58E-06	1.63E-06	1.03E-06	6.49E-07
6,7-dihydro-5-methyl-5H-cyclopentapyrazine	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03	1.69E-03
phenylacetic acid	2.40E-13	1.52E-13	9.56E-14	6.03E-14	3.81E-14	2.40E-14	1.52E-14	9.56E-15	6.03E-15	3.81E-15	2.40E-15
4-methyl-5-hydroxyethyl-thiazole	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05	1.78E-05
o-aminoacetophenone	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04	5.15E-04
nonanoic acid	7.22E-11	4.56E-11	2.88E-11	1.81E-11	1.14E-11	7.22E-12	4.56E-12	2.88E-12	1.81E-12	1.14E-12	7.22E-13
benzoic acid	6.14E-13	3.88E-13	2.45E-13	1.54E-13	9.74E-14	6.14E-14	3.88E-14	2.45E-14	1.54E-14	9.74E-15	6.14E-15
octanoic acid	4.73E-11	2.99E-11	1.88E-11	1.19E-11	7.50E-12	4.73E-12	2.99E-12	1.88E-12	1.19E-12	7.50E-13	4.73E-13
p-menthenethiol	2.00E-02	1.00E-02	7.06E-03	4.46E-03	2.82E-03	1.78E-03	1.12E-03	7.10E-04	4.48E-04	2.83E-04	1.78E-04
methyl quinoxaline	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04	4.32E-04
2-isopentyl-3,6-dimethyl pyrazine	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03	6.09E-03
hydrocinnamic acid	4.11E-13	2.59E-13	1.64E-13	1.03E-13	6.51E-14	4.11E-14	2.59E-14	1.64E-14	1.03E-14	6.51E-15	4.11E-15
4-methylthiazole	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02
methyl anthranilate	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04	3.93E-04
decanoic acid	9.23E-11	5.82E-11	3.67E-11	2.32E-11	1.46E-11	9.23E-12	5.82E-12	3.67E-12	2.32E-12	1.46E-12	9.23E-13
cinnamic acid	8.87E-13	5.59E-13	3.53E-13	2.23E-13	1.41E-13	8.87E-14	5.59E-14	3.53E-14	2.23E-14	1.41E-14	8.87E-15
p-coumaric acid	1.78E-19	7.09E-20	2.82E-20	1.12E-20	4.48E-21	1.78E-21	7.10E-22	2.83E-22	1.12E-22	4.48E-23	1.78E-23
undecylic acid	1.16E-10	7.29E-11	4.60E-11	2.90E-11	1.83E-11	1.16E-11	7.29E-12	4.60E-12	2.90E-12	1.83E-12	1.16E-12
(E)-2-hexenoic acid	5.64E-11	3.56E-11	2.24E-11	1.42E-11	8.93E-12	5.64E-12	3.56E-12	2.24E-12	1.42E-12	8.93E-13	5.64E-13
oleic acid	4.05E-11	2.56E-11	1.61E-11	1.02E-11	6.42E-12	4.05E-12	2.56E-12	1.61E-12	1.02E-12	6.42E-13	4.05E-13
lauric acid	1.42E-10	8.96E-11	5.65E-11	3.57E-11	2.25E-11	1.42E-11	8.96E-12	5.65E-12	3.57E-12	2.25E-12	1.42E-12
phenol	1.31E-05	8.26E-06	5.22E-06	3.30E-06	2.08E-06	1.31E-06	8.30E-07	5.24E-07	3.30E-07	2.09E-07	1.32E-07
guaiacol	3.93E-05	2.49E-05	1.57E-05	9.93E-06	6.27E-06	3.96E-06	2.50E-06	1.58E-06	9.95E-07	6.28E-07	3.96E-07
p-cresol	3.06E-05	1.94E-05	1.23E-05	7.79E-06	4.93E-06	3.11E-06	1.96E-06	1.24E-06	7.83E-07	4.94E-07	3.12E-07
m-cresol	2.19E-05	1.39E-05	8.78E-06	5.55E-06	3.50E-06	2.21E-06	1.40E-06	8.82E-07	5.56E-07	3.51E-07	2.22E-07
3-ethylphenol	2.56E-05	1.62E-05	1.03E-05	6.49E-06	4.10E-06	2.59E-06	1.63E-06	1.03E-06	6.51E-07	4.11E-07	2.59E-07
o-cresol	2.85E-05	1.81E-05	1.15E-05	7.26E-06	4.59E-06	2.90E-06	1.83E-06	1.16E-06	7.29E-07	4.60E-07	2.90E-07
p-vinylguaiacol	5.30E-06	3.35E-06	2.11E-06	1.33E-06	8.42E-07	5.31E-07	3.35E-07	2.12E-07	1.33E-07	8.42E-08	5.31E-08
4-propyl-guaiacol	1.64E-04	1.04E-04	6.58E-05	4.16E-05	2.63E-05	1.66E-05	1.05E-05	6.62E-06	4.18E-06	2.64E-06	1.66E-06
syringol	4.46E-08	2.81E-08	1.78E-08	1.12E-08	7.07E-09	4.46E-09	2.82E-09	1.78E-09	1.12E-09	7.07E-10	4.46E-10
4-vinylphenol	1.68E-06	1.06E-06	6.71E-07	4.24E-07	2.67E-07	1.69E-07	1.06E-07	6.72E-08	4.24E-08	2.68E-08	1.69E-08

Table S2a. SPARC estimated pH dependent n-octanol/water partitioning coefficients (D_{ow}) for ionizable aroma compounds from the Flavornet database.

pH	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	5.5	6.0	6.5	7.0	7.5	8.0	8.5	9.0	9.5	10.0	10.5	11.0	11.5	12.0	12.5	13.0	13.5	14.0
trimethylamine	-1.78	-1.78	-1.78	-1.78	-1.78	-1.78	-1.78	-1.78	-1.78	-1.78	-1.78	-1.78	-1.77	-1.73	-1.64	-1.43	-1.09	-0.67	-0.22	0.18	0.49	0.66	0.73	0.75	0.76	0.76	0.76	0.76	0.76
methanethiol	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.58	0.57	0.54	0.44	0.24	-0.11	-0.54	-1.02	-1.51	-2.01	-2.51	-3.01	-3.51
pyrrolidine	-1.89	-1.89	-1.89	-1.89	-1.89	-1.89	-1.89	-1.89	-1.89	-1.89	-1.89	-1.89	-1.89	-1.89	-1.88	-1.86	-1.79	-1.64	-1.35	-0.96	-0.52	-0.11	0.19	0.36	0.44	0.46	0.47	0.47	0.47
propanoic acid	-0.45	-0.45	-0.45	-0.45	-0.45	-0.46	-0.46	-0.48	-0.53	-0.65	-0.90	-1.28	-1.73	-2.21	-2.71	-3.20	-3.69	-4.15	-4.55	-4.82	-4.97	-5.03	-5.05	-5.05	-5.06	-5.06	-5.06	-5.06	-5.06
butyric acid	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.21	0.16	0.04	-0.21	-0.59	-1.04	-1.53	-2.02	-2.51	-3.00	-3.46	-3.85	-4.12	-4.26	-4.32	-4.34	-4.34	-4.34	-4.35	-4.35	-4.35	-4.35
acetic acid	-0.95	-0.95	-0.95	-0.95	-0.95	-0.95	-0.96	-0.97	-1.02	-1.14	-1.38	-1.75	-2.20	-2.68	-3.18	-3.67	-4.16	-4.61	-5.00	-5.26	-5.40	-5.45	-5.47	-5.48	-5.48	-5.48	-5.48	-5.48	-5.48
methylbutenthiol	2.28	2.28	2.28	2.28	2.28	2.28	2.28	2.28	2.28	2.28	2.28	2.28	2.28	2.28	2.28	2.28	2.27	2.26	2.22	2.12	1.91	1.55	1.11	0.64	0.14	-0.36	-0.85	-1.35	-1.85
pyridine	-2.88	-2.84	-2.74	-2.51	-2.16	-1.71	-1.24	-0.76	-0.29	0.11	0.39	0.54	0.60	0.62	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63
methyl pyrazine	-1.70	-1.21	-0.73	-0.29	0.06	0.28	0.39	0.42	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44
isovaleric acid	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.73	0.68	0.56	0.31	-0.07	-0.52	-1.01	-1.50	-1.99	-2.48	-2.94	-3.33	-3.60	-3.74	-3.80	-3.82	-3.82	-3.83	-3.83	-3.83	-3.83	-3.83
methylfuranthiol	2.04	2.04	2.04	2.04	2.04	2.04	2.04	2.04	2.03	2.03	2.02	1.99	1.90	1.71	1.38	0.95	0.48	-0.02	-0.51	-1.01	-1.51	-2.01	-2.49	-2.95	-3.33	-3.60	-3.73	-3.78	-3.80
methylbutyric acid	0.92	0.92	0.92	0.92	0.92	0.92	0.91	0.90	0.84	0.71	0.46	0.07	-0.38	-0.87	-1.36	-1.86	-2.35	-2.83	-3.26	-3.60	-3.80	-3.89	-3.92	-3.93	-3.93	-3.93	-3.93	-3.93	-3.93
dimethylthiazole	0.79	0.80	0.80	0.82	0.88	1.01	1.26	1.59	1.88	2.05	2.13	2.16	2.17	2.17	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18
o-picoline	-2.61	-2.60	-2.57	-2.47	-2.27	-1.92	-1.49	-1.01	-0.53	-0.05	0.39	0.75	0.98	1.09	1.13	1.14	1.14	1.15	1.15	1.15	1.15	1.15	1.15	1.15	1.15	1.15	1.15	1.15	1.15
methyltetrahydrofuranthiol	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.68	0.63	0.51	0.26	-0.12	-0.57	-1.05	-1.55	-2.05	-2.55	-3.05	-3.55	-4.05
2,5-dimethyl pyrazine	-1.81	-1.32	-0.83	-0.34	0.12	0.50	0.77	0.90	0.95	0.97	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98
2,6-dimethyl pyrazine	-1.90	-1.41	-0.91	-0.43	0.03	0.43	0.72	0.86	0.92	0.94	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95
2-ethyl pyrazine	-1.15	-0.66	-0.18	0.26	0.61	0.83	0.93	0.96	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98
caproic acid	1.54	1.54	1.54	1.54	1.54	1.54	1.53	1.52	1.47	1.35	1.10	0.72	0.27	-0.22	-0.71	-1.20	-1.69	-2.14	-2.51	-2.76	-2.88	-2.93	-2.95	-2.95	-2.95	-2.95	-2.95	-2.95	-2.95
pentanoic acid	0.90	0.90	0.90	0.90	0.90	0.90	0.89	0.88	0.83	0.71	0.46	0.08	-0.37	-0.86	-1.35	-1.84	-2.33	-2.78	-3.17	-3.43	-3.56	-3.61	-3.63	-3.63	-3.64	-3.64	-3.64	-3.64	-3.64
2,3-dimethyl pyrazine	-1.82	-1.33	-0.83	-0.35	0.11	0.50	0.76	0.89	0.94	0.96	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97
fufuryl mercaptan	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.50	1.48	1.41	1.25	0.95	0.54	0.08	-0.41	-0.91	-1.41	-1.91	-2.41	-2.91	-3.41
acetylpyrroline	-0.46	-0.46	-0.46	-0.46	-0.46	-0.46	-0.46	-0.46	-0.46	-0.46	-0.46	-0.45	-0.43	-0.36	-0.25	-0.14	-0.07	-0.04	-0.03	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02
methoxymethylbutanethiol	1.88	1.88	1.88	1.88	1.88	1.88	1.88	1.88	1.88	1.88	1.88	1.88	1.88	1.88	1.88	1.88	1.87	1.86	1.81	1.68	1.43	1.05	0.60	0.11	-0.38	-0.88	-1.38	-1.88	-2.38
ethyl mercaptopropionate	1.62	1.62	1.62	1.62	1.62	1.62	1.62	1.62	1.62	1.62	1.62	1.62	1.62	1.62	1.61	1.58	1.49	1.30	0.97	0.54	0.06	-0.43	-0.93	-1.42	-1.92	-2.42	-2.92	-3.42	-3.91
4,5-dimethyl thiazole	0.79	0.80	0.81	0.86	0.97	1.20	1.52	1.83	2.03	2.12	2.15	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17
hexanethiol	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.15	3.14	3.11	3.03	2.83	2.50	2.07	1.60	1.10	0.61	0.11	-0.39	-0.89
2-methyl-4,5-dihydro-3-furanthiol	2.13	2.13	2.13	2.13	2.13	2.13	2.13	2.13	2.13	2.13	2.11	2.08	1.97	1.75	1.40	0.95	0.47	-0.02	-0.52	-1.02	-1.51	-2.01	-2.49	-2.93	-3.28	-3.50	-3.60	-3.64	-3.65
4-methyl-3-thiazoline	-0.73	-0.73	-0.73	-0.73	-0.73	-0.72	-0.72	-0.72	-0.70	-0.65	-0.53	-0.29	0.03	0.35	0.56	0.66	0.69	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71
2-ethylpyridine	-2.22	-2.20	-2.16	-2.06	-1.83	-1.47	-1.02	-0.54	-0.06	0.42	0.86	1.22	1.44	1.54	1.58	1.59	1.60	1.60	1.60	1.60	1.60	1.60	1.60	1.60	1.60	1.60	1.60	1.60	1.60
3-mercapto-4-methyl-2-pentanone	1.73	1.73	1.73	1.73	1.73	1.73	1.73	1.73	1.73	1.73	1.73	1.73	1.73	1.73	1.73	1.72	1.70	1.63	1.47	1.17	0.76	0.29	-0.20	-0.69	-1.19	-1.69	-2.19	-2.69	-3.19
3-mercaptothiophene	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.52	2.50	2.43	2.27	1.97	1.56	1.10	0.61	0.11	-0.39	-0.89	-1.38	-1.87	-2.32	-2.71	-2.97	-3.10	-3.15	-3.17	-3.17	-3.18	-3.18
2,5-dimethyl-3-furanthiol	2.54	2.54	2.54	2.54	2.54	2.54	2.54	2.54	2.54	2.54	2.53	2.51	2.46	2.33	2.07	1.68	1.23	0.74	0.24	-0.25	-0.75	-1.25	-1.74	-2.21	-2.62	-2.92	-3.08	-3.15	-3.17
3-mercapto-3-methyl-1-butanol	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.11	1.09	1.06	0.95	0.73	0.37	-0.07	-0.55	-1.05	-1.54	-2.04	-2.54	-3.04
2-ethyl-5-methyl pyrazine	-1.29	-0.79	-0.30	0.19	0.64	1.03	1.29	1.42	1.47	1.49	1.49	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50
2,4,5-trimethylthiazole	1.37	1.37	1.37	1.37	1.38	1.41	1.49	1.68	1.96	2.27	2.49	2.61	2.65	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67	2.67
2,3,5-trimethylpyrazine	-2.00	-1.52	-1.03	-0.53	-0.04	0.43	0.85	1.16	1.34	1.42	1.44	1.45	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46
2-acetylpyridine	-2.22	-1.99	-1.63	-1.20	-0.73	-0.29	0.09	0.33	0.45	0.50	0.51	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52
5-methyl-2-furfurylthiol	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.98	1.97	1.92	1.81	1.57	1.20	0.75	0.27	-0.23	-0.72	-1.22	-1.72	-2.22	-2.72
2-acetylthiazole	-0.81	-0.70	-0.48	-0.14	0.21	0.49	0.65	0.71	0.73	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74
2-propionyl-1-pyrroline	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.26	0.28	0.32	0.41	0.51	0.57	0.60	0.61	0.61	0.61	0.61	0.61	0.61	0.61	0.61	0.61	0.61	0.61
2-acetyl-1,4,5,6-tetrahydropyridine	-1.52	-1.51	-1.50	-1.48	-1.40	-1.21	-0.89	-0.47	-0.01	0.44	0.82	1.09	1.23	1.28	1.30	1.30	1.31	1.31	1.31	1.31	1.31	1.31	1.31	1.31	1.31	1.31	1.31	1.31	1.31
2-ethyl-6-methylpyrazine	-1.41	-0.91	-0.42	0.07	0.53	0.92	1.20	1.35	1.40	1.42	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43	1.43
2-isobutylthiazole	2.01	2.01	2.02	2.03	2.07	2.18	2.39	2.68	2.96	3.12	3.20	3.23	3.24	3.24	3.24	3.24	3.24	3.24	3.24	3.24	3.24	3.24	3.24	3.24	3.24	3.24	3.24	3.24	3.24
4-mercapto-4-methyl-2-pentanone	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.47	1.44	1.36	1.17	0.85	0.43	-0.04	-0.53	-1.03	-1.53	-2.03	-2.53
2-methyl-3-ethylpyrazine	-1.31	-0.82	-0.33	0.16	0.62	1.00	1.26	1.39	1.44	1.46	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47
2-methyl-3-thiophenethiol	3.06	3.06	3.06	3.06	3.06	3.06	3.06	3.06	3.05	3.03	2.96	2.80	2.50	2.10	1.63	1.14	0.64	0.15	-0.35	-0.85	-1.33	-1.78	-2.16	-2.42	-2.54	-2.59	-2.60	-2.61	-2.61
5-isopropyl-2-methylpyrazine	-0.86	-0.37	0.12	0.61	1.06	1.45	1.70	1.83	1.88	1.90	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91
2-methoxy-3,6-dimethylpyrazine	-1.51	-1.01	-0.52	-0.04	0.39	0.74	0.94	1.04	1.07	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09
5-ethyl-2,4-dimethylthiazole	1.99	1.99	1.99	2.00	2.00	2.03	2.10	2.27	2.54	2.83	3.05	3.17	3.21	3.23	3.23	3.23	3.23	3.23	3.23	3.23	3.23	3.23	3.23	3.23	3.23	3.23	3.23	3.23	3.23
2,5-dimethyl-3-ethylpyrazine	-1.52	-1.04	-0.55	-0.06	0.43	0.90	1.32	1.63	1.81	1.88	1.91	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92
thenylthiol	2.51	2.51	2.51	2.51	2.51	2.51	2.51	2.51	2.51	2.51	2.51	2.51	2.51	2.51	2.51	2.50	2.47	2.38	2.19	1.87	1.44	0.97	0.47	-0.02	-0.52	-1.02	-1.52	-2.02	-2.52
2-ethyl-3,5-dimethylpyrazine	-1.52	-1.04	-0.54	-0.05	0.44	0.91	1.33	1.65	1.82	1.90	1.92	1.93	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94
2,3-dimethyl-6-ethylpyrazine	-1.51	-1.02	-0.53	-0.04	0.45	0.92	1.34	1.65	1.83	1.90	1.93	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94
2-ethyl-3,5-dimethylpyrazine	-1.52	-1.04	-0.54	-0.05	0.44	0.91	1.33	1.65	1.82	1.90	1.92	1.93	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94
2-isopropyl-3-methoxypyrazine	-0.31	0.18	0.65	1.06	1.36	1.53	1.60	1.62	1.63	1.63	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64	1.64

2-ethenyl-3,5-dimethylpyrazine	-0.95	-0.46	0.04	0.53	0.99	1.39	1.68	1.83	1.89	1.91	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92	1.92
2-acetyl-2-thiazoline	-1.72	-1.72	-1.72	-1.72	-1.71	-1.70	-1.67	-1.59	-1.41	-1.10	-0.75	-0.44	-0.25	-0.17	-0.14	-0.13	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12
2-acetyl-3,4,5,6-tetrahydropyridine	0.38	0.38	0.38	0.38	0.38	0.38	0.38	0.38	0.38	0.38	0.38	0.39	0.41	0.46	0.55	0.65	0.71	0.74	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75
4-mercapto-4-methyl-2-pentanol	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.39	1.35	1.25	1.02	0.67	0.23	-0.26	-0.75	-1.25	-1.75	-2.25	-2.75	
5-methyl-5(H)-cyclopentapyrazine	-1.26	-0.76	-0.27	0.22	0.68	1.07	1.34	1.48	1.54	1.56	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57
3,5-diethyl-2-methylpyrazine	-0.95	-0.47	0.03	0.52	1.01	1.48	1.90	2.20	2.38	2.45	2.47	2.48	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49	2.49
2,3-diethyl-5-methylpyrazine	-0.97	-0.48	0.01	0.50	0.99	1.46	1.88	2.19	2.36	2.44	2.46	2.47	2.47	2.48	2.48	2.48	2.48	2.48	2.48	2.48	2.48	2.48	2.48	2.48	2.48	2.48	2.48	2.48	2.48	2.48
2-sec-butyl-3-methoxypyrazine	0.20	0.69	1.15	1.56	1.85	2.00	2.07	2.09	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10
2-phenylethylthiol	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.88	2.86	2.81	2.68	2.43	2.04	1.59	1.10	0.61	0.11	-0.39	-0.89	-1.39	
2-ethenyl-3-ethyl-5-methylpyrazine	-0.50	0.00	0.49	0.98	1.44	1.84	2.12	2.27	2.33	2.35	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36
2-pentylpyridine	-0.53	-0.52	-0.49	-0.41	-0.22	0.11	0.53	1.01	1.49	1.97	2.41	2.76	2.98	3.09	3.12	3.14	3.14	3.14	3.14	3.14	3.14	3.14	3.14	3.14	3.14	3.14	3.14	3.14	3.14	3.14
2-isobutyl-3-methoxypyrazine	0.21	0.70	1.17	1.58	1.89	2.07	2.14	2.17	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18	2.18
isobutyric acid	0.42	0.42	0.42	0.42	0.42	0.42	0.41	0.39	0.34	0.21	-0.05	-0.43	-0.88	-1.37	-1.86	-2.36	-2.85	-3.31	-3.73	-4.03	-4.19	-4.26	-4.28	-4.29	-4.29	-4.29	-4.29	-4.29	-4.29	
benzothiazole	0.66	0.85	1.14	1.46	1.69	1.80	1.85	1.86	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87
3-mercapto-1-hexanol-1-acetate	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.64	2.64	2.64	2.63	2.60	2.52	2.34	2.01	1.59	1.11	0.62	0.13	-0.37	-0.87	-1.37	-1.87	
6,7-dihydro-5-methyl-5H-cyclopentapyrazine	-0.88	-0.39	0.10	0.57	0.99	1.30	1.47	1.54	1.57	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58
phenylacetic acid	1.03	1.03	1.03	1.03	1.03	1.03	1.02	0.99	0.90	0.70	0.37	-0.06	-0.54	-1.03	-1.53	-2.02	-2.49	-2.93	-3.27	-3.48	-3.58	-3.61	-3.62	-3.63	-3.63	-3.63	-3.63	-3.63	-3.63	
4-methyl-5-hydroxyethyl-thiazole	-0.19	-0.18	-0.15	-0.08	0.10	0.38	0.70	0.95	1.09	1.14	1.16	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17	1.17
o-aminoacetophenone	-0.48	-0.13	0.30	0.73	1.09	1.33	1.44	1.48	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50
nonanoic acid	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.36	3.31	3.19	2.94	2.56	2.11	1.62	1.13	0.64	0.16	-0.28	-0.63	-0.85	-0.95	-0.99	-1.00	-1.00	-1.00	-1.01	-1.01	-1.01	-1.01	
benzoic acid	1.55	1.55	1.55	1.55	1.55	1.54	1.52	1.44	1.27	0.96	0.54	0.07	-0.42	-0.92	-1.42	-1.92	-2.42	-2.91	-3.39	-3.83	-4.19	-4.42	-4.52	-4.56	-4.57	-4.58	-4.58	-4.58	-4.58	
octanoic acid	2.78	2.78	2.78	2.78	2.78	2.78	2.77	2.76	2.71	2.58	2.33	1.96	1.50	1.02	0.53	0.03	-0.45	-0.89	-1.25	-1.48	-1.58	-1.62	-1.64	-1.64	-1.64	-1.64	-1.64	-1.64	-1.64	
p-menthenethiol	4.19	4.19	4.19	4.19	4.19	4.19	4.19	4.19	4.19	4.19	4.19	4.19	4.19	4.19	4.19	4.19	4.18	4.18	4.16	4.10	3.96	3.69	3.30	2.84	2.35	1.86	1.36	0.86	0.36	
methyl quinoxaline	0.04	0.52	0.99	1.39	1.67	1.82	1.88	1.90	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91	1.91
2-isopentyl-3,6-dimethyl pyrazine	-0.19	0.28	0.77	1.27	1.76	2.23	2.65	2.96	3.13	3.21	3.23	3.24	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25	3.25
hydrocinnamic acid	1.67	1.67	1.67	1.67	1.67	1.67	1.66	1.64	1.57	1.41	1.12	0.71	0.25	-0.24	-0.73	-1.22	-1.70	-2.14	-2.49	-2.71	-2.80	-2.84	-2.85	-2.86	-2.86	-2.86	-2.86	-2.86	-2.86	
4-methylthiazole	0.16	0.19	0.27	0.45	0.75	1.09	1.37	1.53	1.59	1.62	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63
methyl anthranilate	-0.50	-0.09	0.35	0.76	1.09	1.28	1.36	1.39	1.40	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41
decanoic acid	3.92	3.92	3.92	3.92	3.92	3.91	3.91	3.89	3.84	3.72	3.47	3.09	2.64	2.16	1.66	1.17	0.70	0.26	-0.09	-0.30	-0.39	-0.43	-0.44	-0.44	-0.45	-0.45	-0.45	-0.45	-0.45	
cinnamic acid	2.50	2.50	2.50	2.50	2.50	2.49	2.47	2.41	2.25	1.96	1.56	1.10	0.64	0.22	-0.11	-0.30	-0.38	-0.41	-0.42	-0.42	-0.42	-0.42	-0.42	-0.42	-0.42	-0.42	-0.42	-0.42	-0.42	
p-coumaric acid	1.78	1.78	1.78	1.78	1.78	1.77	1.76	1.72	1.61	1.38	1.03	0.59	0.12	-0.32	-0.69	-0.94	-1.09	-1.24	-1.49	-1.85	-2.30	-2.78	-3.27	-3.77	-4.27	-4.77	-5.26	-5.75	-6.21	
undecylic acid	4.44	4.44	4.44	4.44	4.44	4.44	4.43	4.41	4.37	4.24	3.99	3.61	3.16	2.68	2.19	1.69	1.22	0.78	0.44	0.24	0.15	0.11	0.10	0.10	0.10	0.10	0.10	0.10	0.10	
(E)-2-hexenoic acid	2.21	2.21	2.21	2.21	2.21	2.21	2.19	2.15	2.04	1.81	1.45	1.00	0.53	0.08	-0.32	-0.60	-0.75	-0.81	-0.83	-0.83	-0.84	-0.84	-0.84	-0.84	-0.84	-0.84	-0.84	-0.84	-0.84	
oleic acid	7.15	7.15	7.15	7.15	7.15	7.15	7.14	7.13	7.08	6.95	6.70	6.32	5.87	5.39	4.89	4.41	3.94	3.52	3.21	3.03	2.96	2.93	2.92	2.92	2.92	2.92	2.92	2.92	2.92	
lauric acid	4.95	4.95	4.95	4.95	4.95	4.95	4.95	4.93	4.88	4.76	4.51	4.13	3.68	3.19	2.70	2.21	1.74	1.30	0.97	0.77	0.68	0.65	0.64	0.64	0.63	0.63	0.63	0.63	0.63	
phenol	1.61	1.61	1.61	1.61	1.61	1.61	1.61	1.61	1.61	1.61	1.61	1.61	1.61	1.61	1.61	1.61	1.60	1.59	1.56	1.47	1.26	0.92	0.49	0.01	-0.48	-0.98	-1.48	-1.98	-2.48	
guaiacol	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.75	1.75	1.74	1.70	1.60	1.38	1.02	0.58	0.10	-0.39	-0.89	-1.39	-1.89	-2.39	
p-cresol	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.20	2.20	2.18	2.14	2.01	1.76	1.39	0.94	0.45	-0.04	-0.54	-1.04	-1.54	
m-cresol	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.21	2.20	2.20	2.17	2.10	1.94	1.64	1.22	0.76	0.27	-0.23	-0.73	-1.23	-1.73	
3-ethylphenol	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.75	2.74	2.72	2.65	2.48	2.18	1.77	1.30	0.81	0.32	-0.18	-0.68	-1.18	
o-cresol	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.82	1.81	1.80	1.76	1.65	1.42	1.05	0.61	0.13	-0.37	-0.87	-1.36	-1.86	
p-vinylguaiacol	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.65	2.64	2.64	2.64	2.64	2.63	2.59	2.49	2.27	1.91	1.47	0.99	0.50	0.00	-0.50	-1.00	-1.50	-2.00	
4-propyl-guaiacol	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.37	3.35	3.30	3.17	2.90	2.51	2.05	1.57	1.07	0.58	0.08	-0.42	
syringol	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.15	1.14	1.09	0.96	0.71	0.33	-0.13	-0.61	-1.11	-1.60	-2.10	-2.60	-3.10	-3.60	
4-vinylphenol	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.55	2.54	2.53	2.50	2.40	2.19	1.85	1.41	0.93	0.44	-0.06	-0.56	-1.05	-1.55	-2.05	