Supporting Information — "Odour emissions from poultry litter – A review litter properties, odour formation and odorant emissions from porous materials"

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Table S1. Selected odorants and other relevant compounds from meat chicken excreta, litter and/or housing.
Table includes identification information, chemical properties, odour thresholds and odour character.
References are in square brackets [ ].
Odour thresholds are presented in units of ppb and µg/m³. Values with adjoining reference are the source value and corresponding value in alternate units have been calculated.
Compounds with reference 'unpublished data' are suspected to occur in meat chicken odour based on unpublished information
n/a = 'not available'

Odorant	Alternative names	Molecular weight [34]	CAS No.[34]	Formula	Odour Character	Odour Threshold (min) (µg/m³)	Odour Threshold (max) (µg/m³)	Odour Threshold (min) (ppbv)	Odour Threshold (max) (ppbv)	Henry's constant at 25°C (M/atm) [34]	Log_{10} Hcc at 25°C (dimension-less)	Vapour Pressure at 25°C (kPa) [34]	Water solubility at 25°C (mg/L)[32]	References (reported from meat chickens)
Acids & Esters														
Acetic acid	Ethanoic acid	60.052	64-19-7	$C_2H_4O_2$ or CH_3COOH	Vinegar [46]	25 [35] (892) (1180) (2500 [43])	2.5×10^5 [43] (1.0×10^4 [35])	10.2 (363 [44]) (480 [18]) (1018)	1.02×10^5 (4071)	6300	-5.19	2.1	1,044,600	[19; 29; 50; 52; 57]; 'Poultry' litter [53]
Methylacetate	Acetic acid methyl ester; methyl acetate	74.0785	79-20-9	CH_3OCOCH_3 or $C_3H_6O_2$	Fruity, solvent, sweet [55]; ether-like [6]	500 [35] (1.39×10^4)	5.5×10^5 [35]	165 (4600 [18])	1.82×10^5	9.133	-2.35	28.8	243500 (@20°C)	unpublished data
Propanoic acid	Propionic acid; Methyl acetic acid	74.0785	79-09-4	CH_3CH_2COOH or $C_3H_6O_2$	Pungent, disagreeable, rancid odour [6]; sour, mildly cheese-like [32]	84[43] (108) (485)	6.0×10^4 [43]	27.7 (35.5 [44]) (160 [18])	1.98×10^4	5950	-5.16	0.47 [32]	1,000,000	[50; 52; 57]
Ethyl acetate	Acetic acid ethyl ester; Ethylacetate; Ethyl ethanoate	88.1051	141-78-6	$CH_3OCOC_2H_5$ or $C_4H_8O_2$	Ether-like, fruity [6]; fruity with a brandy note, reminiscent of pineapple [32]	600 [35] (3135) (3603) (9477)	1.8×10^5 [35]	166.5 (870 [31]) (1000 [18]) (2630 [44])	5.0×10^4	6.15	-2.18	12.6	80,100	[29; 57]
Butanoic acid	*n*-butyric acid; butyric acid	88.1051	107-92-6	C_3H_7C00H or $C_4H_8O_2$	Unpleasant, rancid, obnoxious [32]	0.4 [35] (0.69) (3.6) (14))	4.2×10^4 [35]	0.11 (0.19 [31]) (1.0 [18]) (3.9 [44])	1.17×10^4	4700	-5.06	0.15	60,000	[19; 29; 50; 52; 57]; 'poultry' [35]
2-methyl-propanoic acid	Isobutyric acid; isobutanoic acid; 2-methylpropanoic acid	88.1051	79-31-2	$(CH_3)_2C_2H_3COOH$ or $C_4H_8O_2$	Sharp, butter-fat-like odour, like butyric acid but not as unpleasant [32]	5 [35] (5.4) (70.3)	330 [35]	1.38 (1.5 [31]) (19.5 [44])	91.6	1100	-4.43	0.24 [32]	167,000 (@20°C)	[50; 52; 57]
n-propyl-acetate	Acetic acid, propyl ester	102.1317	109-60-4	$CH_3OCOC_3H_7$ or $CH_3COOCH_2CH_2CH_3$ or $C_5H_{10}O_2$	Mild fruity [6]; pleasant, odour of pears [32]	200 (2800)	7.0×10^4	48 (670 [18])	1.68×10^4	4.5	-2.04	4.78 [32]	18,900 (@20°C)	unpublished data
Butanoic acid, methyl ester	n-butyric acid, methyl ester; Methyl butyrate methyl butanoate	102.1317	623-42-7	$CH_3CH_2CH_2COOCH_3$ or $C_5H_{10}O_2$	Apple-like [32]	20 [23]	n/a	4.8	n/a	4.8	-2.07	4.25	15,000	unpublished data
3-methylbutanoic acid	Isovaleric acid; Isobutylformic acid; 3 methylbutyric acid	102.1317	503-74-2	$(CH_3)_2C_2H_3COOH$ or $C_5H_{10}O_2$	Unpleasant [38]; rancid-cheese [32]; body odour [24]	0.2 [35] (0.33) (2.5)	10.3 (6.9 [35])	0.05 (0.08 [31]) (0.6 [38])	2.5 [44] (1.65)	1200	-4.47	0.06 [32]	40,700 (@20°C)	[50; 52]

Table S1 cont'd

Odorant	Alternative names	Molecular weight [34]	CAS No.[34]	Formula	Odour Character	Odour Threshold (min) (μg/m³)	Odour Threshold (max) (μg/m³)	Odour Threshold (min) (ppbv)	Odour Threshold (max) (ppbv)	Henry's constant at 25°C (M/atm) [34]	Log_{10} Hcc at 25°C (dimension-less)	Vapour Pressure at 25°C (kPa) [34]	Water solubility at 25°C (mg/L)[32]	References (reported from meat chickens)
2-methyl butanoic acid	2-methylbutyric acid	102.1317	116-53-0	$C_2H_5CH(CH_3)COOH$ or $C_5H_{10}O_2$	Irritant, stench [44]	7.8	20 [35]	1.9 [44]	4.8	n/a	n/a	n/a	n/a	unpublished data
Pentanoic Acid	Valeric acid; n-pentanoic acid; n-valeric acid; propylacetic acid;1-butanecarboxylic acid	102.1317	109-52-4	$CH_3(CH_2)_3COOH$ or $C_5H_{10}O_2$	Unpleasant, similar to butyric acid [32]	0.16 (0.8 [35]) (20.0)	120 [35]	0.04 [31] (0.19) (4.8 [44])	28.7	2200	-4.73	0.026 [32]	24,000	[50; 52; 57]
Propanoic acid, propyl ester	Propionic acid, propyl ester; Propyl propionate	116.1583	106-36-5	$CH_3CH_2COOCH_2CH_3$ or $C_6H_{12}O_2$	n/a	17.3	n/a	5.7[31]	n/a	2.6	-1.8	1.85	n/a	unpublished data
Butanoic acid, ethyl ester	n-butyric acid, ethyl ester; Ethyl butyrate	116.1583	105-54-4	$CH_3CH_2CH_2C(O)OC_2H_5$ or $C_6H_{12}O_2$	Fruity odour with pineapple undernote [32]	n/a	n/a	n/a	n/a	2.8	-1.84	2.30	4900 (@20°C)	unpublished data
Hexanoic Acid	Caproic acid; n-Caproic acid; n-Hexanoic acid; Butylacetic acid	116.1583	142-62-1	$CH_3(CH_2)_4COOH$ or $C_6H_{12}O_2$	Characteristic goat-like [32]	2.9 (20 [35])	520 [35] (59.8)	0.6 [31] (4.2)	109.5 (12.6 [44])	1300	-4.50	0.006 [32]	10,300	[50; 52; 57]
Benzoic acid	Benzenecarboxylic acid	122.1213	65-85-0	C_6H_5C00H or $C_7H_6O_2$	Slight benzaldehyde odour (almonds), faint, pleasant [32]	n/a	n/a	n/a	n/a	14,000	-5.53	0.0001 [32]	3400	[50]
Butanoic acid, propyl ester	n-butyric acid, propyl ester; Propyl butyrate	130.1849	105-66-8	$CH_3CH_2CH_2COOCH_2CH_2CH_3$ or $C_7H_{14}O_2$	n/a	n/a	n/a	n/a	n/a	1.9	-1.67	0.79	n/a	unpublished data
Heptanoic acid	Enanthic acid; n-Heptanoic acid; Heptoic acid; Oenanthic acid	130.1849	111-14-8	$CH_3(CH_2)_5COOH$ or $C_7H_{14}O_2$	Disagreeable, rancid, tallow-like [32]	22 [35]	146.4 (33 [35])	4.1	27.5 [44] (6.2)	2965	-4.86	0.001 [32]	2820	[50; 52]
Butanoic acid, butyl ester	n-butyric acid, butyl ester; Butyl Butyrate	144.2114	109-21-7	$CH_3CH_2CH_2COO(CH_2)_3CH_3$ or $C_8H_{16}O_2$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	unpublished data
Butanoic acid, 1-methylpropyl ester	butyric acid, sec-butyl ester; butanoic acid, 2-butyl ester	144.2114	819-97-6	$C_8H_{16}O_2$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	unpublished data
Dimethyl itaconate	Butanedioic acid, methylene-, dimethyl ester;	158.1519	617-52-7	$CH_3O_2CCH_2C(=CH_2)CO_2CH_3$ or $C_7H_{10}O_4$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[50]
Benzoic acid, 4-ethoxy-,ethyl ester	Ethyl 4-ethoxybenzoate; Ethyl para-ethoxybenzoate	194.2271	23676-09-7	$C_{11}H_{14}O_3$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	0.0 [41]	n/a	[29]
Diethyl-phthalate	Anozol; Phthalol; solvanol; Diethyl ester of Phthalic acid; Neantine	222.2372	84-66-2	C_6H_4-1,2-$(CO_2C_2H_5)_2$ or $C_{12}H_{14}O_4$	Very slight, aromatic, practically odourless[32]	n/a	n/a	n/a	n/a	1200	-4.47	0.0003 [32]	1080	[29]
Triethyl Citrate	Citric acid, triethyl ester; 1,2,3-propanetricarboxylic acid, 2-hydroxy-, triethyl ester	276.2830	77-93-0	$HOC(COOC_2H_5)(CH_2COOC_2H_5)_2$ or $C_{12}H_{20}O_7$	n/a	n/a	n/a	n/a	n/a	2.6×10^5 [41]	-6.8	0.0003	65,000	[50]

Table S1 cont'd

Odorant	Alternative names	Molecular weight [34]	CAS No.[34]	Formula	Odour Character	Odour Threshold (min) (µg/m³)	Odour Threshold (max) (µg/m³)	Odour Threshold (min) (ppbv)	Odour Threshold (max) (ppbv)	Henry's constant at 25°C (M/atm) [34]	Log_{10} Hcc at 25°C (dimension-less)	Vapour Pressure at 25°C (kPa) [34]	Water solubility at 25°C (mg/L)[32]	References (reported from meat chickens)
1-Octadecanesulfonyl chloride	Octadecane-1-sulphonyl chloride	353.0032	10147-41-8	$C_{18}H_{37}ClO_2S$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	3.18×10^{-8} [41]	n/a	[29]
Alcohols														
Methanol	Methyl alcohol; carbinol	32.0419	67-56-1	CH_3OH or CH_4O	Alcoholic, pungent [32]	3931 (4.3×10^4)	1.9×10^5	3000 [18] (3.3×10^4 [31])	1.4×10^5 [44]	220	-3.73	16.9	1,000,000	[19; 50]
Ethanol		46.068	64-17-5	CH_3CH_2OH or C_2H_6O	Mild, pleasant, wine-like (vinous), whisky-like, ethereal, [32]	0.64 [35]	1350 [35]	340	7.16×10^5	198	-3.68	7.8	1,000,000	[7; 19; 50]
i-Propanol	Isopropanol; Isopropyl alcohol; sec-Propyl alcohol; dimethylcarbinol; 2-Propanol	60.0950	67-63-0	$(CH_3)_2CHOH$ or C_3H_8O	Pleasant, mixture of ethanol and acetone [32]	3900 [35] (7840 [43]) (2.5×10^4) (5.4×10^4)	5.4×10^6 [35] (4.9×10^5 [43])	1585 (3190) (1.02×10^4 [44]) (2.2×10^4 [18])	2.2×10^6 (2.0×10^5)	125	-3.48	6.05 [32]	1,000,000	[7; 19]
1-propanol	Propyl alcohol; *n*-propyl alcohol; *n*-propanol; propanol	60.0950	71-23-8	$CH_3CH_2CH_2OH$ or C_3H_8O	Alcohol-like [6]; similar to ethanol	75 [35] (231) (6390)	1.4×10^5 [35]	30.5 (94 [31]) (2600 [18])	5.7×10^4	143.3	-3.54	2.81	1,000,000	[7; 50]; 'Poultry' litter [53]
2-butanol	sec-butanol; sec-butyl alcohol	74.1216	78-92-2	$CH_3CH(OH)CH_2CH_3$ or $C_4H_{10}O$	Strong pleasant [6]; wine like odour, sweet [32]	400 [35] (667) (7580)	8×10^4 [35]	132 (220 [31]) (2500 [18])	2.64×10^4	103.5	-3.40	2.43	181,000	[29]
1-butanol	*n*-butyl alcohol; n-butanol; butanol	74.123	71-36-3	$CH_3(CH_2)_3OH$ or C_4H_9OH	Solvent [36]; alcohol [21]; harsh fusel odour with banana (banana liqueur), amyl alcohol, sweet, rancid [32]	158 [35] (1485)	42,000 [35]	52.1 (490 [44])	13,854	125.0	-3.48	0.72	63,200	[7; 29; 30; 36; 50]
2-methyl-3-buten-2-ol	Dimethylvinylcarbinol; dimethylvinylmethanol	86.1323	115-18-4	$CH_2=CHC(CH_3)_2OH$ or $C_5H_{10}O$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	3.13 [32]	190,000 (@20°C)	unpublished data
3-methyl-1-butanol	Isoamyl alcohol; *i*-pentanol; isopentyl alcohol	88.148	123-51-3	$C_5H_{12}O$ or $(CH_3)_2CHCH_2CH_2OH$	Disagreeable [6]	80 [35] (3.6×10^4 [43])	1.26×10^5 [43] (161) (151)	22.19 (9985)	3.49×10^4 (44.7 [44]) (42 [18])	70.9 [41]	-3.24	0.32 [32]	26,700	[29]
1-pentanol	n-pentanol; pentyl alcohol, n-amyl alcohol, n-pentyl alcohol	88.1482	71-41-0	$CH_3(CH_2)_4OH$ or $C_5H_{12}O$	Fusel-like, mild [32]	360.5 (756 [43])	1658	100 [31] (209)	460 [18]	76	-3.27	0.29	22,000	[30]
4-hydroxy-4-methyl-2-pentanone	Diacetone alcohol; Tyranton; Acetonyldimethylcarbinol	116.1583	123-42-2	$(CH_3)_2C(OH)CH_2COCH_3$ or $C_6H_{12}O_2$	Faint, pleasant, minty [32]	1344 [43]	4.8×10^5 [43]	282.9	1.01×10^5	n/a	n/a	0.17	1,000,000	[29; 30]
2-Butoxy-ethanol	Butyl glycol; Ethylene glycol butyl ether; 2-n-butoxyethanol	118.1742	111-76-2	$CH_3(CH_2)_3OCH_2CH_2OH$ or $C_6H_{14}O_2$	Mild, ether-like, slightly rancid, pleasant, sweet [32]	208	483	43 [31]	100 [18]	625	-4.18	0.12 [32]	1,000,000	[30]

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1-Octen-3-ol	Amyl vinyl carbinol; 3-Hydroxy-1-octene; Vinyl hexanol; Matsuica alcohol; mushroom alcohol	128.2120	3391-86-4	$CH_3(CH_2)_4CH(OH)CH=CH_2$ or $C_8H_{16}O$	n/a	2.7 [29]	n/a	0.515	n/a	n/a	n/a	n/a	n/a	[29]
2-ethyl-1-hexanol	2-Ethylhexanol	130.2279	104-76-7	$C_4H_9CH(C_2H_5)CH_2OH$ or $C_8H_{18}0$	Mild, oily, slightly floral odour reminiscent of rose [32]; musty [43]	400 [35]	734 [43]	75.1	137.8	n/a	n/a	0.02	880	[29; 30]
Aldehydes														
Acetaldehyde	Ethanal	44.053	75-07-0	C_2H_4O or CH_3CHO	Fruity [46]; sweet fruity [9]; yoghurt, sweet burning [55]	0.2 [43] (2.7 [35])	4140 [43]	0.11 (1.5)	2397	14	-2.53	120	1,000,000	[19] ; 'Poultry' litter [53]; poultry [35]
Acetone	2-propanone	58.079	67-64-1	$(CH_3)_2CO$	Solvent, sweet [36]; nail polish	940 [35] (4.75×10^4 [43])	1.61×10^6 [43] (1.55×10^6 [35]) (3.08×10^4)	58.1 (2.0×10^4)	6.79×10^5 (6.53×10^5) (1.3×10^4 [18])	28.13	-2.84	32.8	1,000,000	[7; 19; 30; 36; 50]; 'Poultry' litter [53]
Butanal	Butyraldehyde; 1-butanal; Butyric aldehyde; *n*-butanal; butylaldehyde	72.1057	123-72-8	$CH_3CH_2CH_2CHO$ or C_4H_8O	Pungent, aldehyde odour [32]; sweet, rancid [43]	0.84 [35] (1.96 [31]) (13.6 [43]) (26.3)	2.6×10^4 [43] (200 [35])	0.285 (0.67) (4.6) (8.9 [44])	9,000 (67.8)	9.6	-2.37	14.8	71,000	[57]
2-Butanone	Methyl ethyl ketone; butanone; MEK	72.106	78-93-3	$C_2H_5COCH_3$ or C_4H_8O	Sweet, minty [38]; acetone-like [6]	737.3 [43]	2.50×10^5 [35] (1.48×10^5 [43])	250	8.48×10^4 (5.0×10^4)	20	-2.69	12.08 [32]	223,000	[7; 19; 29; 50; 57]; 'Poultry' litter [53]
Methylhydrazone acetaldehyde	Acetaldehyde, N-methylhydrazone, AMFH; 1-Ethylidene-2-methylhydrazine	72.1090	17167-73-6	$C_3H_8N_2$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	4.8 [41]	n/a	[30]
2,3-butanedione	Diacetyl	86.089	431-03-8	$CH_3COCOCH_3$ or $C_4H_6O_2$	Butter, rancid, fat [36]; quinone, chlorine-like [32]; yoghurt, sour cream, sour milk [16]	0.007 [35] (0.18) (3.5 [43]) (5.0 [35]) (15.4)	88.0 [43] (26.0)	0.002 (0.05 [31]) (0.99) (1.42) (4.37 [42])	25.0 (7.39 [42])	65.50	-3.2	7.67	200 (@20°C)	[29; 36; 50]
3-methyl-butanal	Isovaleraldehyde; Isopenanal; Isovaleric aldehyde	86.132	590-86-3	$C_5H_{10}O$ or $(CH_3)_2CHCH_2CHO$	Malt, rancid [36]; apple-like, acrid [32]	1.6 [35] (7.8 [44])	8.1 [29]	0.45 (2.2)	2.3	2.46 [41]	-1.78	6.67 [32]	1400 (@20°C)	[29; 30; 36]
2-pentanone	Ethyl acetone; methyl propyl ketone	86.1323	107-87-9	$CH_3COCH_2CH_2CH_3$ or $C_5H_{10}O$	Acetone-like [6]	3.88×10^4	n/a	1.1×10^4 [18]	n/a	12.37	-2.48	4.72 [32]	43,000	[50]

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3-pentanone	Diethyl ketone; DEK; ethyl Ketone; Methacetone; 1,3-Dimethylacetone; Ethyl propionyl; pentan-3-one; Diethylcetone; Pentanone-3	86.1323	96-22-0	$C_5H_{10}O$	Acetone-like [32]	1,090	n/a	310 [18]	n/a	20	-2.69	5.02 [32]	45,890	[50]
Pentanal	n- Valeraldehyde ; Valeraldehyde; n-Pentenal; valeric aldehyde; amyl aldehyde; Pentalaldehyde	86.1323	110-62-3	$CH_3(CH_2)_3CHO$ or $C_5H_{10}O$	Powerful, acrid, pungent [32]	1.44	31.7	0.41 [31]	9.0 [44]	6.6	-2.20	3.4 [32] (@20°C)	11,700	[29]
3-hydroxy-2-butanone	Acetoin; Dimethylketol; Acetyl-methyl-carbinol	88.105	513-86-0	$C_4H_8O_2$ or $CH_3COCH(OH)CH_3$	Mushroom, earth [36]; buttery; woody, yoghurt [32]; butter-like [44]	n/a	n/a	n/a	n/a	n/a	n/a	2.7 [32]	1,000,000	[29; 36; 50]
4-methyl-3-penten-2-one	Mesityl oxide; Isopropylidene-Acetone; Isobutenyl methyl ketone; isopropylideneacetone	98.1430	141-79-7	$(CH_3)_2C=CHCOCH_3$ or $C_6H_{10}O$	Spearmint, peppermint, honey-like [32]	68.8 [43]	1.0×10^5 [43]	16.9	2.49×10^4	27.2 [41]	-2.82	1.46	28,900 @ 20°C	[30]
Hexanal	Caproaldehyde, Caproic aldehyde; n-hexanal	100.1589	66-25-1	$CH_3(CH_2)_4CHO$ or $C_6H_{12}O$	Fruity; green grass [32]; grassy [24]	n/a	n/a	n/a	n/a	4.9	-2.08	1.51 (@30°C)	5640	[7; 29; 30; 57]; Layer manure [24]
4-Methylpentan-2-one	Methyl isobutyl ketone MIK; MIBK;; isopropylacetone	100.1589	108-10-1	$C_6H_{12}O$ or $(CH_3)_2CHCH_2COCH_3$	Pleasant, ketonic, camphor [32]	410 [43] (696) (2200)	1.93×10^5 [43]	100 (170 [31]) (537 [44])	4.7×10^4	2.4	-1.77	2.62	19,000	[50]
Benzaldehyde	Benzenecarbonal, benzoic aldehyde, phenylmethanal	106.1219	100-52-7	C_6H_5CH0 or C_7H_6O	Almond-like, oil of bitter almonds [32]; onion, burnt food [24]	0.8 [43]	182 [43]	0.184	42	39	-2.98	0.17	6950	[29; 30; 50; 57]; 'Poultry' litter[53]
2-n-Butylacrolein	2-methylene-hexanal; 2-Butylacrolein	112.1696	1070-66-2	$C_7H_{12}O$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	0.89 [41]	n/a	[30]
Heptanal	Oenanthaldehyde	114.186	111-71-7	$C_7H_{14}O$ or $C_6H_{13}CHO$	Rancid, citrus [36]; fatty, pungent, fruity [32]; green, soapy, stink bug, nuts [16]	6 [35] (14 [43])	260 [35] (93.2 [43])	1.3 (3.0)	55.7 (20.0)	3.50	-1.93	0.38 [32]	1250	[29; 30; 36; 57]
Acetophenone	Methyl phenyl ketone; acetylbenzene; 1-phenylethanone	120.1485	98-86-2	$CH_3COC_6H_5$ or C_8H_8O	Pungent odour of acacia, orange blossom or jasmine-like [32]; almond, sweet [43]	10 [35] (19.7) (835 [43]) (1500 [35])	2946 [43]	2.0 (4.0 [18]) (170) (305)	600	110	-3.43	0.05	6130	[29; 50; 57]
6-Methyl-5-hepten-2-one	Methylheptenone; Sulcatone	126.1962	110-93-0	$(CH_3)_2C=CHCH_2CH_2COCH_3$ or $C_8H_{14}O$	Powerful, fatty, green, citrus [32]	n/a	n/a	n/a	n/a	n/a	n/a	n/a	0 (insoluble)	[30]

Table S1 cont'd

Odorant	Alternative names	Molecular weight [34]	CAS No.[34]	Formula	Odour Character	Odour Threshold (min) (µg/m³)	Odour Threshold (max) (µg/m³)	Odour Threshold (min) (ppbv)	Odour Threshold (max) (ppbv)	Henry's constant at 25°C (M/atm) [34]	Log_{10} Hcc at 25°C (dimension-less)	Vapour Pressure at 25°C (kPa) [34]	Water solubility at 25°C (mg/L)[32]	References (reported from meat chickens)
Octanal	Caprylaldehyde; caprylic aldehyde	128.212	124-13-0	$C_8H_{16}O$ or $C_7H_{15}CHO$	Green, citrus [36]; soapy, fatty, cardboard, metallic [16]	0.7 [12] (1.4 [12])	7.8 [35]	0.13 (0.27)	1.5	2.00	-1.69	0.16 [32]	560	[30; 36]
2-ethyl-hexanal	Butylethylacetyaldehyde; 2-ethylhexaldehyde	128.2120	123-05-7	$CH_3(CH_2)_3CH(C_2H_5)CHO$ or $C_8H_{16}O$	Mild [32]	n/a	n/a	n/a	n/a	1.3 [41]	-0.51	0.27 [32]	700 (@20°C)	[29; 30]
3,5-dimethyl-benzaldehyde	m-Xylene-5-carboxaldehyde	134.1751	5779-95-3	$(CH_3)_2C_6H_3CHO$ or $C_9H_{10}O$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	unpublished data
2,5-Dimethyl-benzaldehyde	Isoxylaldehyde	134.1751	5779-94-2	$(CH_3)_2C_6H_3CHO$ or $C_9H_{10}O$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[29]
Nonanal	*n*-nonaldehyde; Perlargonaldehyde; nonyl aldehyde	142.2386	124-19-6	$CH_3(CH_2)_7CHO$ or $C_9H_{18}O$	Orange-rose odour, floral, waxy, green [32]; moldy-cellar-earthy, cardboard, fruity, dusty, goat stable, fatty, old chair/house [16]	0.3 [35] (1.0 [12]) (2.5 [12]) (13.0)	45 [35]	0.052 (0.172) (0.43) (2.24 [44])	7.74	1.0	-1.39	0.05	96	[29]
1,3-diphenyl-2-propen-1-one	Chalcone	208.2552	94-41-7	$C_6H_5CH{=}CHCOC_6H_5$ or $C_{15}H_{12}O$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	unpublished data
Fixed Gasses														
Ammonia		17.031	7664-41-7	NH_3	Ammonia, pungent [21];	26.6 [38]	37,800 [35]	38	5.43×10^4	67.8	-3.22	994.4	310,000–480,000	[1; 2; 5; 10; 11; 14; 15; 20; 22; 25-27; 33; 37; 39; 40; 48; 49; 54; 58; 59]
Hydrogen Sulfide		34.081	7783-06-4	H_2S	Decaying vegetation[21]; Rotten eggs[28; 47];	0.21 [56] 0.7 [43]	24.9 [51] (14 [43])	0.502	17.9 (10.04)	0.10	-0.39	2032	insoluble	[51]
Sulfur dioxide	Sulphurous acid anhydride; sulphurous anhydride; SO_2;	64.0638	7446-09-5	O_2S	Strong, suffocating, irritating, pungent [32]	870 [35] (1175 [43]) (2280)	3816	332 (448) (870 [31])	1.0×10^5 [35]	1.33	-1.51	401.2	107,000 @ 21°C	[30]
Hydrocarbons														
Propene	Propylene; methylethylene	42.0797	115-07-1	$CH_3CH{=}CH_2$ or C_3H_6	Aromatic [32; 43]	2.2×10^4 (3.96×10^4 [43]) (9.0×10^4)	1.3×10^5 (1.16×10^5 [43])	1.3×10^4 [31] (2.3×10^4) (5.2×10^4 [44])	7.6×10^4 [18] (6.7×10^4)	0.006	0.85	1160 [32]	200	[50]
2-Methyl-1-propene	Isobutylene; Isobutene; 1,1-Dimethylethylene; 2-Methylpropene	56.1063	115-11-7	$(CH_3)_2C{=}CH_2$ or C_4H_8	Coal gas odour [32]	2.8×10^4	4.58×10^4 [43]	1.2×10^4 [18]	2.0×10^4	0.0046	0.95	307.7 [32]	236	[50]
Chloroethane	Aethylis, Chlorethyl; Chlorene; Monochloroethane	64.514	75-00-3	C_2H_5Cl	Ethereal, pungent, ether-like [32]	n/a	n/a	n/a	n/a	0.084	-0.31	161 [41]	5680 (@20°C)	[50]

Table S1 cont'd

Odorant	Alternative names	Molecular weight [34]	CAS No.[34]	Formula	Odour Character	Odour Threshold (min) (µg/m³)	Odour Threshold (max) (µg/m³)	Odour Threshold (min) (ppbv)	Odour Threshold (max) (ppbv)	Henry's constant at 25°C (M/atm) [34]	Log_{10} Hcc at 25°C (dimension-less)	Vapour Pressure at 25°C (kPa) [34]	Water solubility at 25°C (mg/L)[32]	References (reported from meat chickens)
Cyclopentane	Pentamethylene	70.1329	287-92-3	C_5H_{10}	Mild, sweet [32]	n/a	n/a	n/a	n/a	0.006	0.8	42.3	156 [41]	[50]
Pentane	*n*-pentane	72.1488	109-66-0	CH_3 $[CH_2]_3CH_3$ or C_5H_{12}	Petrol-like [6]	4130 (6600 [43]) (1.18×10^6) (3.5×10^5 [35])	3×10^6 [43]	1400 [31] (2236) (4.00×10^5 [18]) (1.19×10^5)	1.02×10^6	0.0008	1.72	68.3	38	[29; 50] ; 'Poultry' litter [53]
Benzene		78.112	71-43-2	C_6H_6	Sweet, solvent [36]; solventy [28]; aromatic, petrol-like [32]	1495 (4500 [43])	3.80×10^5 [35] (2.7×10^5 [43])	468 [18] (1408)	1.19×10^5 (8.45×10^4)	0.17	-0.62	12.6	1790	[7; 29; 30; 36; 50]; 'Poultry' litter [53];
methylcyclopentane	Methyl-cyclopentane; methylpentamethylene	84.1595	96-37-7	$C_5H_9CH_3$ or C_6H_{12}	Petrol-like [32]	n/a	n/a	n/a	n/a	0.0028	1.16	18.3	42	[30]
Dichloromethane	Methylene chloride;	84.933	75-09-2	CH_2Cl_2	Chloroform-like, sweet, pleasant [32]	8.6×10^4 (9.8×10^4)	5.6×10^5	2.5×10^4 [18] (2.8×10^4 [44])	1.6×10^5 [31]	0.36	-0.94	57.2	13,000	[7; 50]
Acetic acid, ethenyl ester	Vinyl acetate; acetic acid vinyl ester; Ethenyl acetate[32]	86.0892	108-05-4	$CH_3CO_2CH=CH_2$ or $C_4H_6O_2$	Sweetish smelling (@ low conc.), sharp and irritating (@ high conc.) [32]	360 [43]	1760	102.2	500 [18]	1.7	-1.62	15.3	20,000 @ 20°C	[30]
3-Methyl-pentane	3-methylpentane	86.1745	96-14-0	C_6H_{14}	Petrol-like [6]	3.14×10^4	n/a	8900 [31]	n/a	0.0006	1.84	25.3	17.9	[7]
2-Methyl-pentane	2-methylpentane; isohexane	86.1754	107-83-5	$(CH_3)_2CHC_3H_7$ or C_6H_{14}	Petrol-like [6]	289[43]	2.47×10^4	81.9	7000 [31]	0.0006	1.83	28.2	14	[7]
Hexane	*n*-hexane	86.1754	110-54-3	$CH_3(CH_2)_4CH_3$ or C_6H_{14}	Petrol-like [6]	5290	2.8×10^5 (2.3×10^5 [35])	1500 [31]	8.0×10^4 [18] (6.5×10^4)	0.0006	1.83	20.1	9.5	[29]
Toluene		92.138	108-88-3	$C_6H_5CH_3$ or C_7H_8	Sweet, solvent [36]; strong, fruity [32]	600 [56]	5.9×10^5 [56]	159	1.57×10^5	0.15	-0.56	3.8	526	[29; 30; 36; 50; 57]; 'Poultry' litter [53]
1,3,5-cycloheptatriene	Cycloheptatriene; Tropilidene	92.1384	544-25-2	C_7H_8	n/a	n/a	n/a	n/a	n/a	0.21	-0.71	3.13	n/a	[30]
Phenol	Carbolic acid	94.1112	108-95-2	C_6H_5OH or C_6H_6O	Phenolic [24]; medicinal, sweet [43]; sweet, tarry [32]	21.5 (178.6 [43])	2.2×10^4 [43]	5.6 [31] (46.4)	5820	2900	-4.85	0.046[32]	82,400	[50; 52; 57]; Layer manure [24]
3-Methylhexane	2-ethylpentane; 2-ethyl-pentane; 3-Methyl-hexane	100.2019	589-34-4	$CH_3CH_2CH_2CH(CH_3)CH_2CH_3$ or C_7H_{16}	Solvent odour [7]	3442	n/a	840 [31]	n/a	0.00042	1.99	n/a	4.95 [41]	[7]
3-hydroxy-3-methyl-2-butanone	dimethylacetylcarbinol	102.1317	115-22-0	$(CH_3)_2C(OH)COCH_3$ or $C_5H_{10}O_2$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	unpublished data
1,3,5,7-cyclooctatetraene	[8]-Annulene; cyclooctatetraene	104.1491	629-20-9	C_8H_8	n/a	n/a	n/a	n/a	n/a	n/a	n/a	1.05	n/a	[29]

Table S1 cont'd

Odorant	Alternative names	Molecular weight [34]	CAS No.[34]	Formula	Odour Character	Odour Threshold (min) (µg/m³)	Odour Threshold (max) (µg/m³)	Odour Threshold (min) (ppbv)	Odour Threshold (max) (ppbv)	Henry's constant at 25°C (M/atm) [34]	Log_{10} Hcc at 25°C (dimension-less)	Vapour Pressure at 25°C (kPa) [34]	Water solubility at 25°C (mg/L)[32]	References (reported from meat chickens)
Styrene	Vinylbenzene; Ethenylbenzene, Styrol, Phenylethylene, Cinnamene	104.1491	100-42-5	$C_6H_5CH=CH_2$ or C_8H_8	Sweet, floral, aromatic, extremely penetrating [32]; solventy, rubbery [43]	149 (170) (430 [43])	8.6×10^5 [43]	35 [31] (40 [18]) (101)	2.02×10^5	0.34	-0.91	0.85 [32]	300	[30]
Xylenes	Dimethyl benzene	106.1650	1330-20-7	$C_6H_4(CH_3)_2$ or C_8H_{10}	n/a	304 (350 [35])	8.6×10^4 [35]	70 [18] (80)	2.0×10^4	0.14 [41]	-0.53 [41]	1.1 [41]	161 [41]	[7]
p-Xylene	p-methyltoluene; 1,4-dimethyl-benzene	106.1650	106-42-3	$C_6H_4(CH_3)_2$ or C_8H_{10}	Sweet, aromatic [32]	251.8 (304)	2127.6	58 [31] (70 [18])	490 [44]	0.14	-0.52	1.18	162	[29; 30]
1,3-dimethyl-benzene	m-Xylene	106.1650	108-38-3	$C_6H_4(CH_3)_2$ or C_8H_{10}	Sweet, benzene-like, characteristic aromatic [32]	178	304	41 [31]	70 [18]	0.13	-0.50	1.11	161	[29]
Ethylbenzene	Ethylbenol; EB; Phenylethane	106.1650	100-41-4	$C_6H_5C_2H_5$ or C_8H_{10}	Pungent, sweet, petrol-like [32]	12.5 (738) (8700 [43])	8.7×10^5 [43]	2.88 [44] (170 [31]) (2003)	2.0×10^5	0.12	-0.47	1.28 [32]	169	[29; 30]
o-Xylene	1,2-Dimethyl –benzene; o-Dimethylbenzene; 2-Methyltoluene	106.165	95-47-6	$C_6H_4(CH_3)_2$ or C_8H_{10}	Sweet, aromatic [32]	304 (851 [44])	1650	70 [18] (196)	380 [31]	0.2	-0.69	0.88	178	[30]
4-methylphenol	p-Cresol; p-Tolyl alcohol	108.1378	106-44-5	$CH_3C_6H_4OH$ or C_7H_8O	Phenolic, barnyard [24]; sweet, tarry [32]; Faecal [60]	0.239 (2.1 [60])	9.0 [60]	0.054 [31] (0.48)	(2.0)	1300	-4.50	0.015 [32]	21,400	[50; 52; 57]; Layer manure [24]
Benzyl alcohol	Benzenemethanol; phenylcarbinol	108.1378	100-51-6	$C_6H_5CH_2OH$ or C_7H_8O	Faint aromatic [32]	n/a	n/a	n/a	n/a	9000	-5.34	0.013	42,900	[29]
Octane	n-Octane; Methylheptane	114.2285	111-65-9	$CH_3(CH_2)_6CH_3$ or C_8H_{18}	Petrol-like [32]	7940 (2.7×10^4) (7.1×10^4 [35]) (2.24×10^5)	(7.1×10^5 [35])	1700 [31] (5750 [44]) (1.5×10^4) (4.8×10^4 [18])	(1.5×10^5)	0.00034	2.08	1.88 [32]	0.66 [32]	[7]
2-Methylheptane	Dimethylhexane	114.2285	592-27-8	$(CH_3)_2CH(CH_2)_4CH_3$ or C_8H_{18}	n/a	514	n/a	110 [31]	n/a	0.00027	2.18	6.8 [41]	0.0 [32]	[7]
3-Methylheptane	2-Ethylhexane	114.2285	589-81-1	$CH_3(CH_2)_3CH(CH_3)CH_2CH_3$ or C_8H_{18}	n/a	7000	n/a	1500 [31]	n/a	0.00027	2.18	2.6 [41]	0.79 [41]	[7]
2,4-Dimethylhexane	2,4-dimethyl hexane	114.2285	589-43-5	$CH_3CH_2CH(CH_3)CH_2CH(CH_3)_2$ or C_8H_{18}	n/a	n/a	n/a	n/a	n/a	0.00028	2.16	4.04	n/a	[7]
Trichloromethane	Chloroform; Formyl trichloride	119.378	67-66-3	$CHCl_3$	Pleasant, etheric [32]	1.17×10^4 (1.9×10^4) (5.7×10^4) (2.5×10^5 [43])	1.0×10^6 [43]	2400 [18] (3800 [31]) (1.17×10^4 [44]) (5.12×10^4)	2.1×10^5	0.25	-0.92	25.8	7950	[50]

Table S1 cont'd

Odorant	Alternative names	Molecular weight [34]	CAS No.[34]	Formula	Odour Character	Odour Threshold (min) (µg/m³)	Odour Threshold (max) (µg/m³)	Odour Threshold (min) (ppbv)	Odour Threshold (max) (ppbv)	Henry's constant at 25°C (M/atm) [34]	Log_{10} Hcc at 25°C (dimension-less)	Vapour Pressure at 25°C (kPa) [34]	Water solubility at 25°C (mg/L)[32]	References (reported from meat chickens)
Propyl benzene	1-Phenylpropane; Phenylpropane; Isocumene; n-Propylbenzene	120.1916	103-65-1	$C_6H_5CH_2CH_2CH_3$ or C_9H_{12}	n/a	18.7	n/a	3.8 [31]	n/a	0.14	-0.53	0.45 [32]	23.4	[30]
Mesitylene	1,3,5-Trimethylbenzene; Trimethylbenzol	120.1916	108-67-8	$C_6H_3(CH_3)_3$ or C_9H_{12}	Peculiar, aromatic, sweet [32]	835	1131	170 [31]	230 [18]	0.16	-0.58	0.3 [32]	48.2	[30]
4-ethyl-phenol	p-Ethylphenol; Paraethylphenol	122.1644	123-07-9	$C_2H_5C_6H_4OH$ or $C_8H_{10}O$	Burnt, phenolic, medicinal [24]; powerful, woody-phenolic [32]; pungent [60]	3.5 [60]	10 [60]	0.7	2.0	1290 [41]	-4.5	0.005 [32]	4900	[50; 52]; Layer manure [24]
2-methoxy-phenol	Guaiacol	124.1372	90-05-1	$(CH_3O)C_6H_4OH$ or $C_7H_8O_2$	Burnt [24]; sweet, aromatic, slightly phenolic [32]	n/a	n/a	n/a	n/a	900	-4.34	0.014	18,700	[29]; Layer manure [24]
Naphthalene		128.1705	91-20-3	$C_{10}H_8$	Mothballs [32]; tar like [43]	440 (1500 [43])	1.25×10^5 [43]	84 [18] (286)	2.38×10^4	2.4	-1.77	0.011 [32]	31	[29]
Nonane	n-nonane	128.2551	111-84-2	$CH_3(CH_2)_7CH_3$ or C_9H_{20}	Petrol-like [32]	1.15×10^4 (2.47×10^5)	3.4×10^6 [43]	2200 (4.7×10^4 [18])	6.5×10^5 [31]	0.0002	2.31	0.59 [32]	0.22	[30]
4-propylphenol	P-propyl Phenol;	136.1910	645-56-7	$CH_3CH_2CH_2C_6H_4OH$ or $C_9H_{12}O$	n/a	n/a	n/a	n/a	n/a	877	-4.33	0.005 [41]	1280 [41]	[50]
α-pinene	Alpha-pinene	136.234	80-56-8	$C_{10}H_{16}$	Pine [36]; turpentine	2100 [56]	2.3×10^4 [56]	377	4130	0.003 [41]	1.08	0.63 [32]	2.49	[30; 36]
β-pinene	Beta-pinene	136.234	127-91-3	$C_{10}H_{16}$	Earth, mushroom [36];Characteristic turpentine odour, dry, woody, piney, resinous [32]	65 [36]	n/a	1.17×10^4	n/a	0.05	-0.08	0.39	4.89	[36]
D-Limonene	Cyclohexane; Citrene; Carvene;	136.2340	5989-27-5	$C_{10}H_{16}$	Pleasant, lemon-like [32]	10 [35]	n/a	1.8	n/a	0.03 [41]	0.12	0.26	13.8	[7]; 'Poultry' litter [53]
Limonene	Dipentene; citrene; carvene;1-methyl-4-prop-1-en-2-ylcyclohexene;	136.2340	138-86-3	$C_{10}H_{16}$	Pleasant, lemon-like, citrus, penetrating, penetrating [32]	10 [35]	211.7	1.8	38 [31]	0.031 [41]	0.12	0.263 [32]	13.8	[50]
2-Methyl naphthalene	Methyl-2-naphthalene	142.1971	91-57-6	$C_{11}H_{10}$	n/a	58.1 [43]	290.5 [43]	10.0	50.0	2.1	-1.72	0.007 [32]	24.6	[50]
Decane	*n*-Decane	142.2817	124-18-5	$CH_3(CH_2)_8CH_3$ or $C_{10}H_{22}$	n/a	3600	4300	620 [31]	(740 [18; 44])	0.00014	2.47	0.17 [32]	0.052	unpublished data
2-Methyl-nonane	Isoparaffin; iso-decane; 2-Methylnonane	142.2817	871-83-0	$CH_3(CH_2)_6CH(CH_3)_2$ or $C_{10}H_{22}$	n/a	n/a	n/a	n/a	n/a	0.00018		n/a	n/a	[30]
2,4,6-Trimethyl-heptane	2,4,6-Trimethylheptane	142.2817	2613-61-8	$C_{10}H_{22}$	n/a	n/a	n/a	n/a	n/a	0.00018	2.36	n/a	n/a	[30]
1,4-dichloro-benzene	1,4-dichlorobenzene; p-Dichlorobenzene; Paradichlorobenzene	147.002	106-46-7	$C_6H_4Cl_2$	Mothball-like, penetrating [32]; mothballs [43]	1082 (9.0×10^4 [43])	1.8×10^5 [43]	180 [18] (1.5×10^4)	3.0×10^5	0.5	-1.09	0.23 [32]	79	[30]
Undecane	n-Undecane; Hendecane	156.3083	1120-21-4	$CH_3(CH_2)_9CH_3$ or $C_{11}H_{24}$	n/a	5560	7480	870 [31]	1170 [44]	0.0005 [41]	1.9	0.05 [32]	0.044	[30]

Table S1 cont'd

Odorant	Alternative names	Molecular weight [34]	CAS No.[34]	Formula	Odour Character	Odour Threshold (min) (µg/m³)	Odour Threshold (max) (µg/m³)	Odour Threshold (min) (ppbv)	Odour Threshold (max) (ppbv)	Henry's constant at 25°C (M/atm) [34]	Log_{10} Hcc at 25°C (dimension-less)	Vapour Pressure at 25°C (kPa) [34]	Water solubility at 25°C (mg/L)[32]	References (reported from meat chickens)
4-Methyl-decane	4-Methyldecane	156.3083	2847-72-5	$C_{11}H_{24}$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[30]
Tetrachloroethylene	Ankilostin; Ethylene Tetrachloride; Perchlorethylene	165.833	127-18-4	CCl_2=CCl_2 or C_2Cl_4	Ether-like, mild, sweet, chloroform-like [32]; chlorinated solvent [43]	3.14×10^4 [43] (1.83×10^5)	4.69×10^5 [43]	4623 (2.7×10^4 [18])	6.91×10^4	0.058	-0.15	2.46 [32]	206	[30]
2,2,4,6,6-pentamethyl-heptane	Permthyl 99A	170.3348	13475-82-6	$C_{12}H_{26}$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[30]
Dodecane	n-Dodecane	170.3348	112-40-3	$CH_3(CH_2)_{10}CH_3$ or $C_{12}H_{26}$	n/a	766	1.4×10^4	110 [31]	2040 [44]	0.00014	2.47	0.018 [32]	0.0037	[30; 50]
beta-Terpinyl acetate	B-Terpinal acetate; p-Menth-8-en-1-ol, acetate; Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, acetate	196.286	10198-23-9	$C_{12}H_{20}O_2$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[30]
Hexadecane	*n*-hexadecane; cetane; n-cetane	226.4412	544-76-3	$CH_3(CH_2)_{14}CH_3$ or $C_{16}H_{34}$	n/a	n/a	n/a	n/a	n/a	0.0043	0.98	n/a	0.00009	unpublished data
2,2,4,4,6,8,8-Heptamethyl-nonane	Isocetane; HMN;	226.4412	4390-04-9	$(CH_3)_3CCH_2CH(CH_3)CH_2C(CH_3)_2CH_2C(CH_3)_3$ or $C_{16}H_{34}$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[29]
Amines														
Methylamine	MMA	31.057	74-89-5	CH_5N or CH_3NH_2	Fishy [46]; ammonia-like [32]	1.2 [35] (25.2 [43]) (4065)	1.2×10^4 [43] (6100 [35])	0.945 (19.8)	9450 (4802)	36	-2.94	353 [32]	1,250,000	unpublished data
Dimethylamine		45.084	124-40-3	$(CH_3)_2NH$ or C_2H_7N	Ammonia-like, fish-like [6]	84.6 [43]	86.7	45.8	47 [18]	31.0	-2.88	207	163,000 (@40°C)	unpublished data
Trimethylamine	TMA	59.110	75-50-3	$(CH_3)_3N$ or C_3H_9N	Fishy [46]; cat urine [21]; fecal [24]	0.26 [35] (0.8 [43]) (1.064)	2100 [35]	0.11 (0.33) (0.44 [38])	869	9.5	-2.37	215 [32]	89,000 (@30°C)	[36]
Nitrogen containing														
Acetonitrile	Cyanomethane; Ethanenitrile; Methyl Cyanide	41.0519	75-05-8	CH_3CN or C_2H_3N	Aromatic, sweet, ethereal [32]	2.2×10^4 (6.7×10^4) (7.0×10^4 [43])	1.64×10^5	1.3×10^4 [31] (4.2×10^4 [18]) (4.2×10^4)	9.8×10^4 [44]	49	-3.08	11.8	1,000,000	[50]
Acetamide	Acetic acid amide; ethanamide; methanecarboxamide	59.0672	60-35-5	CH_3CONH_2 or C_2H_5NO	Odourless or mousy [32]	n/a	n/a	n/a	n/a	2.3×10^5 [41]	-6.74	0.005 [32]	2,250,000	[50]
2-Methyl-1H-pyrrole	2-methyl-pyrrole	81.1158	636-41-9	C_5H_7N	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[29]
4,5-dimethyloxazole		97.1152	20662-83-3	C_5H_7NO	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[50]
1-methyl-2-pyrrolidinone	M-Pyrol; N-methylpyrrolidione	99.1311	872-50-4	C_5H_9NO	Mild amine [32]	n/a	n/a	n/a	n/a	22,400 [41]	-5.74	0.05 [32]	1,000,000 [41]	[30]

Table S1 cont'd

Odorant	Alternative names	Molecular weight [34]	CAS No.[34]	Formula	Odour Character	Odour Threshold (min) (µg/m³)	Odour Threshold (max) (µg/m³)	Odour Threshold (min) (ppbv)	Odour Threshold (max) (ppbv)	Henry's constant at 25°C (M/atm) [34]	Log_{10} Hcc at 25°C (dimension-less)	Vapour Pressure at 25°C (kPa) [34]	Water solubility at 25°C (mg/L)[32]	References (reported from meat chickens)
Diisopropylamine	N-isopropyl-1-amino-2-methylethane	101.19	108-18-9	$(CH_3)_2CHNHCH(CH_3)_2$ or $C_6H_{15}N$	Ammonia, fish-like [32]	520 [43] (7450)	3400 [43]	125.6 (1800 [18])	821.5	10.4 [41]	-2.41	79.4 [32]	110,000	[30]
Indole	Ketole;	117.1479	120-72-9	C_8H_7N	Faecal [60]	0.15 (1.4)	1.9[60]	0.032 [44] (0.30 [31])	0.40	1890	-4.67	0.0016 [32]	3560	[19; 50]
2,3,5-Trimethyl pyrazine	Trimethylpyrazine	122.1677	14667-55-1	$C_7H_{10}N_2$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[50]
N-Butyl-1-butanamine	N-Dibutylamine;	129.2432	111-92-2	$(CH_3CH_2CH_2CH_2)_2NH$ or $C_8H_{19}N$	Ammonia like [32]; fishy, amine [43]	423[43]	2540[43]	80.1	481	11.0	-2.43	0.34 [32]	3500	[30]
Skatole	3-methyl-indole	131.1745	83-34-1	C_9H_9N	Barnyard [24]; perfume [43]; characteristic fecal (fecal at high concentration and pleasant/sweet at low concentration) [32]	4.0×10^{-4} [43] (0.03) (1.2 [12]) (3.02)	268 [43]	7.5×10^{-5} (0.006 [31]) (0.22) (0.56 [44])	50	n/a	n/a	0.0007 [32]	n/a	[19; 50]; Layer manure [24]; poultry [35]
N,N-dibutyl-formamide	DBF; Dibutylformamide	157.2533	761-65-9	$HCON(CH_2CH_2CH_2CH_3)_2$ or $C_9H_{19}NO$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[29]
Sulfur containing/Thiols														
Methanethiol	Methyl mercaptan; MM	48.107	74-93-1	CH_3SH or CH_4S	Rotten cabbage [38];	0.0003 [56] (0.04 [43]) (2.2 [51])	82 [43]	1.52×10^{-4} (0.02) (1.18)	41.67	0.31	-0.87	196.2	15,400	[19; 51]
Carbonyl sulfide		60.075	463-58-1	COS	Sulfide odour except when pure [32]	70 [56] (135 [51])	180 [56]	28.5 (55.1)	73.3	0.021	0.29	1254.8 [32]	1220	[19; 51]
Dimethyl sulfide	DMS	62.134	75-18-3	C_2H_6S or $(CH_3)_2S$	Rotten eggs [21]; Rotten vegetable (cabbage, canned corn) [47]; wild radish [32]	0.3 [56] (2.5 [43]) (5.6 [51])	160 [56] (50.8 [43])	0.12 (1.0) (2.2)	63.0 (20.0)	0.55	-1.13	66.9	22,000	[19; 29; 51; 57]
Ethanethiol	Ethyl mercaptan	62.134	75-08-1	C_2H_5SH or C_2H_6S	Natural gas [46]; penetrating garlic-like, skunk-like	0.032 [43] (0.043 [56])	92 [43] (21 [56])	0.013 (0.017)	36.2 (8.264)	0.253	-0.79	70.3	15,603	[19]
Carbon disulfide	Methyl disulfide	76.141	75-15-0	CS_2	Herbaceous, cabbage, sweet, vegetable [55]	24.3 [43] (70 [56]) (95.5 [44])	2.3×10^{4} [43] (296.4 [51]) (180 [56])	7.8 (22.5) (30.7)	7418 (95.2) (57.8)	0.055	-0.13	48.1	2160	[19; 30; 50; 51; 57]
1-propanethiol	Propyl mercaptan; n-propylmercaptan; propanethiol	76.161	107-03-9	$CH_3CH_2CH_2SH$ or C_3H_8S	Onion [24]; offensive, characteristic cabbage odour[32]	0.04	3.9	0.013 [31]	1.26 [44]	0.25	-0.79	20.56	1900	[19]; Layer manure [24]
Diethyl sulfide	Ethyl sulfide; sulfodor; ethylthioethane	90.187	352-93-2	$(C_2H_5)_2S$ or $C_4H_{10}S$	Garlic-like, ethereal [32]; Foul, garlicky [43]	0.122 (1.4 [35]) (4.5 [35])	17.7 [43]	0.033 [31] (0.38) (1.22)	4.8	0.56	-1.14	8.31	3130	unpublished data
Dimethyl sulfone	Methyl sulfone; Methylsulfonemethane; MSM; DMSO2	94.1328	67-71-0	$(CH_3)_2SO_2$ or $C_2H_6O_2S$	n/a	n/a	n/a	n/a	n/a	> 50,000	< -6.09	n/a	n/a	[29; 50]

Table S1 cont'd

Odorant	Alternative names	Molecular weight [34]	CAS No.[34]	Formula	Odour Character	Odour Threshold (min) (µg/m³)	Odour Threshold (max) (µg/m³)	Odour Threshold (min) (ppbv)	Odour Threshold (max) (ppbv)	Henry's constant at 25°C (M/atm) [34]	Log_{10} Hcc at 25°C (dimension-less)	Vapour Pressure at 25°C (kPa) [34]	Water solubility at 25°C (mg/L)[32]	References (reported from meat chickens)
Dimethyl disulfide	DMDS	94.199	624-92-0	CH_3SSCH_3 or $C_2H_6S_2$	Purification [13]; putrid [8]; rotten garlic [46]; smoke, burning, rubber [36]; rotten cabbage [47]; intense onion [32]	0.1 [43] (0.3 [12]) (1.1 [56]) (47.5 [51])	346 [43] (78 [56])	0.03 (0.08) (0.29) (12.3)	89.8 (20.2)	0.96	-1.37	3.8	3000 [41]	[7; 19; 29; 30; 36; 50; 51; 57]
Tetrahydrothiophene 1,1-dioxide	Cyclic tetramethylene sulfone; Sulfolane;	120.170	126-33-0	$C_4H_8O_2S$	Odourless [32]	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[50]
Diethyl disulfide	Ethyl disulfide	122.252	110-81-6	$(C_2H_5S)_2$ or $C_4H_{10}S_2$		0.3 [35] (10)	19.5 [43]	0.06 (2.0 [31])	3.9	0.56	-1.14	0.57	n/a	
Dimethyl trisulfide	DMTS	126.264	3658-80-8	$C_2H_6S_3$ or $(CH_3)_2S_3$	Metallic, sulfur, pungent [36]; garlicky [21]; onion [3]	0.06 [56] (6.2 [43]) (7.3 [35])	8.8 [51]	0.012 (1.2) (1.4)	1.7	n/a	n/a	0.15 [41]	2390 [41]	[29; 36; 51] [7; 19; 30]
Unclassified/Other														
Water vapour		18.0153	7732-18-5	H_2O	Odourless					1785	-4.64	3.16		
2-methyl-,1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester propanoic acid	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[29]
1,4-pentadiene	n/a	68.1170	591-93-5	$CH_2=CHCH_2CH=CH$ or C_5H_8	n/a	n/a	n/a	n/a	n/a	0.0084	0.69	96.8	n/a	[30]
R-(–)-1,2-propanediol	(R)-(–)-Propylene glycol, (R)-(–)-Propylene glycerol	76.0944	4254-14-2	$CH_3CH(OH)CH_2OH$ or $C_3H_8O_2$	n/a	n/a	n/a	n/a	n/a	n/a		0.011 [45] (@20°C)	n/a	[29]
6,7-Dimethyl-3H-isobenzofuran-1-one	n/a	162.1852	CID 583914 [32]	$C_{10}H_{10}O_2$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[29]
Diethyl ethylidenemalonate	Propanedioic acid, ethylidene- diethyl ester	186.2051	1462-12-0	$CH_3CH=C(CO_2C_2H_5)_2$ or $C_9H_{14}O_4$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[50]
4,5,6,7-tetramethylphthalide	4,5,6,7-tetramethyl-2(3H)-Benzofuranone	190.238 [41]	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	[29]
Hexamethylcyclotrisiloxane		222.4618	541-05-9	$C_6H_{18}O_3Si_3$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	0.58	n/a	[7]
Octamethylcyclotetrasiloxane		296.6158	556-67-2	$C_8H_{24}O_4Si_4$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	0.14	0.005	[7]

Figure S1.1. Graphical summary of odour threshold values for selected compounds (Table S1)

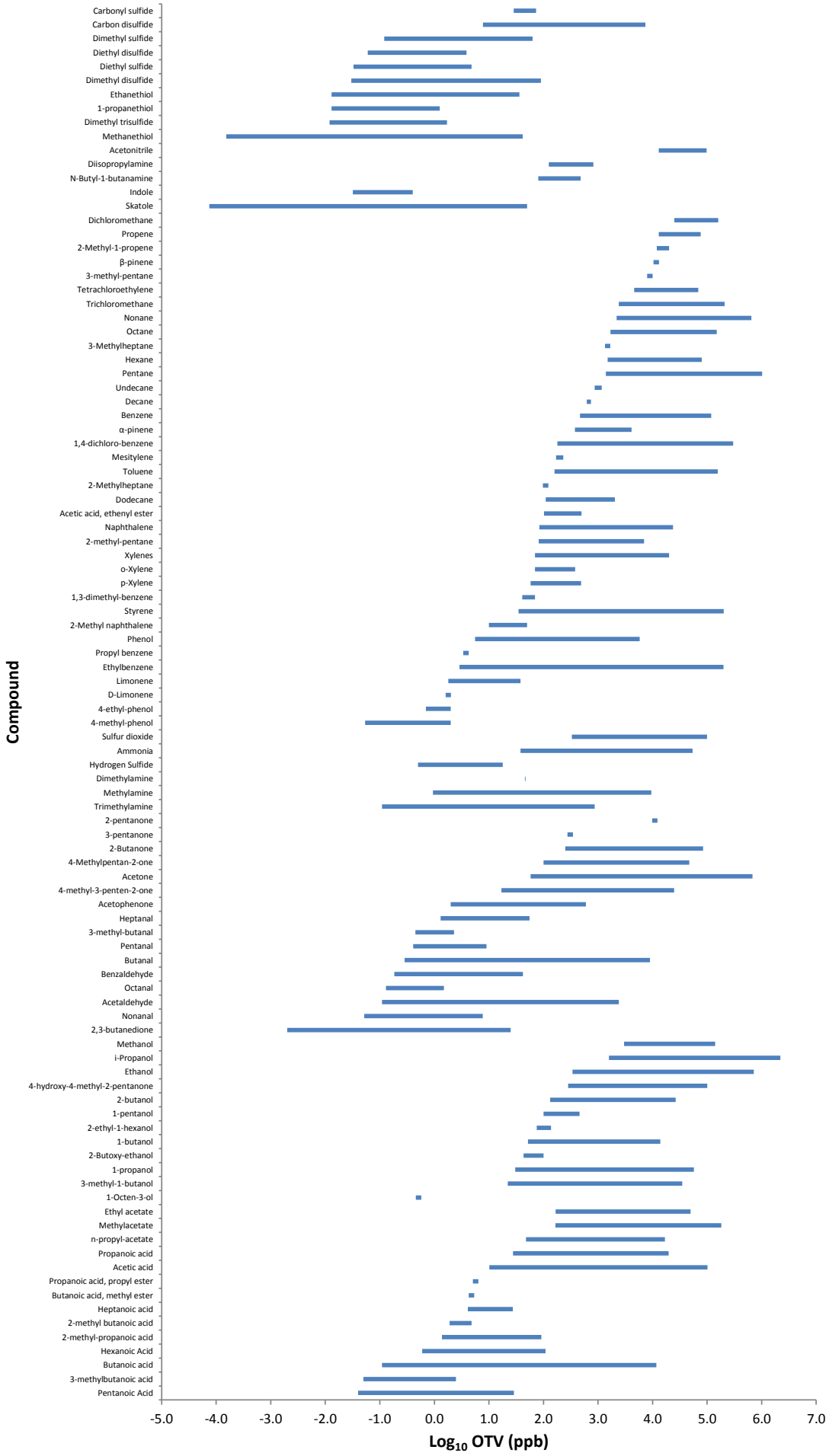


Figure S1.2. Graphical Summary of water solubility for selected compounds (Table S1)

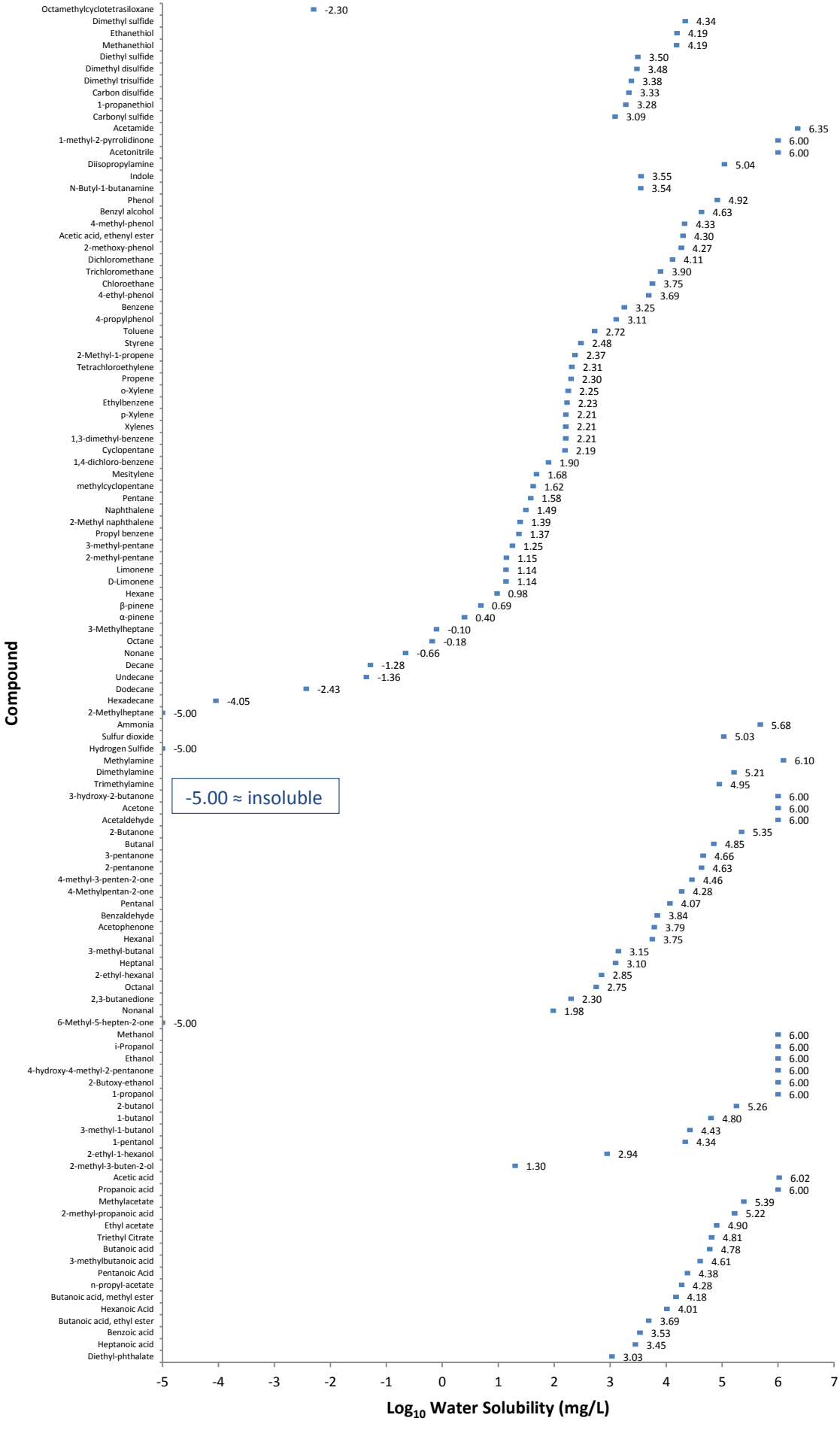


Figure S1.3. Graphical summary of Henry's Law constants for selected compounds (Table S1). Classifications for dependence on gas phase, gas/liquid phase or liquid phase turbulence derived from Hudson and Ayoko (2008)

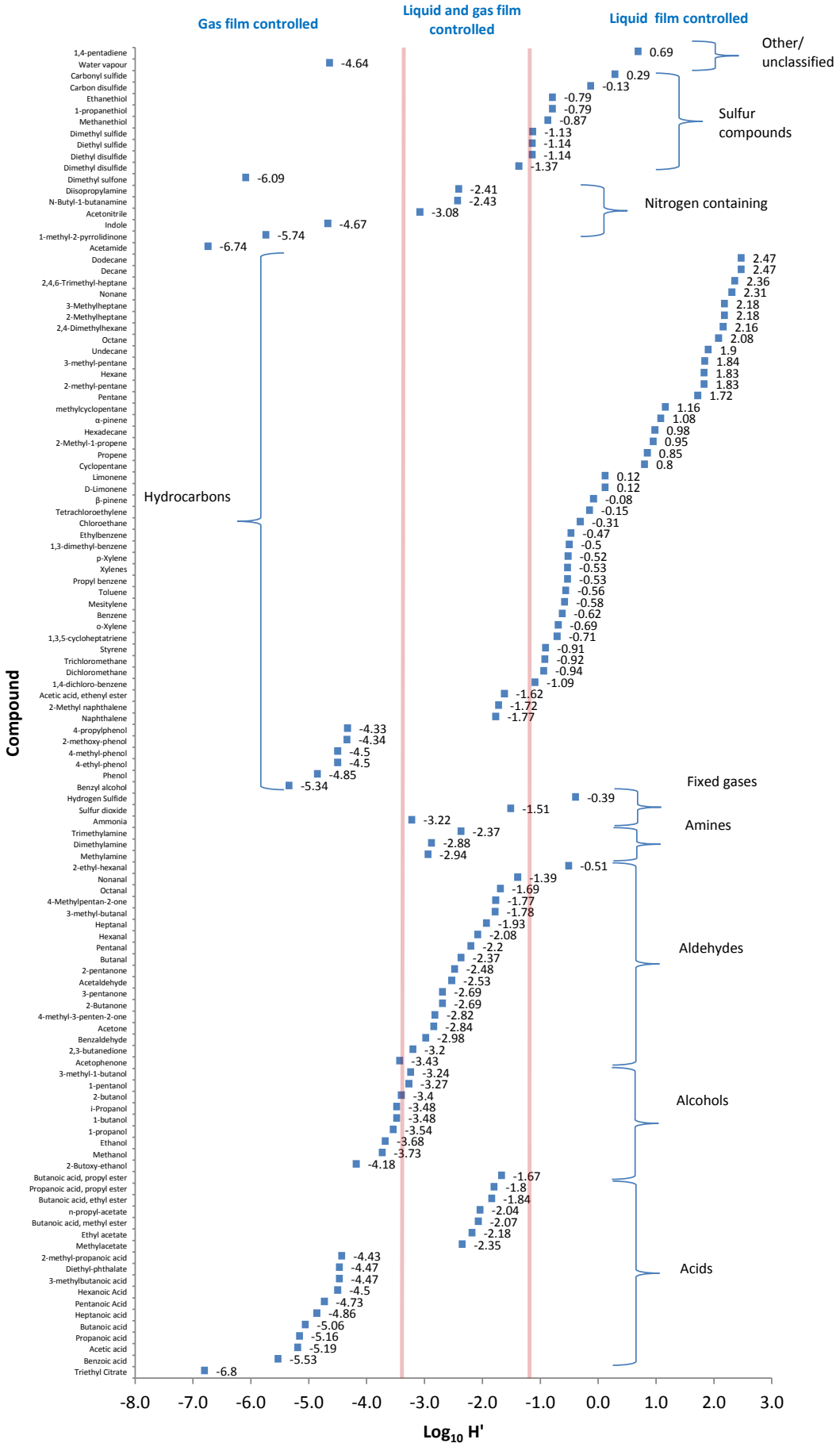
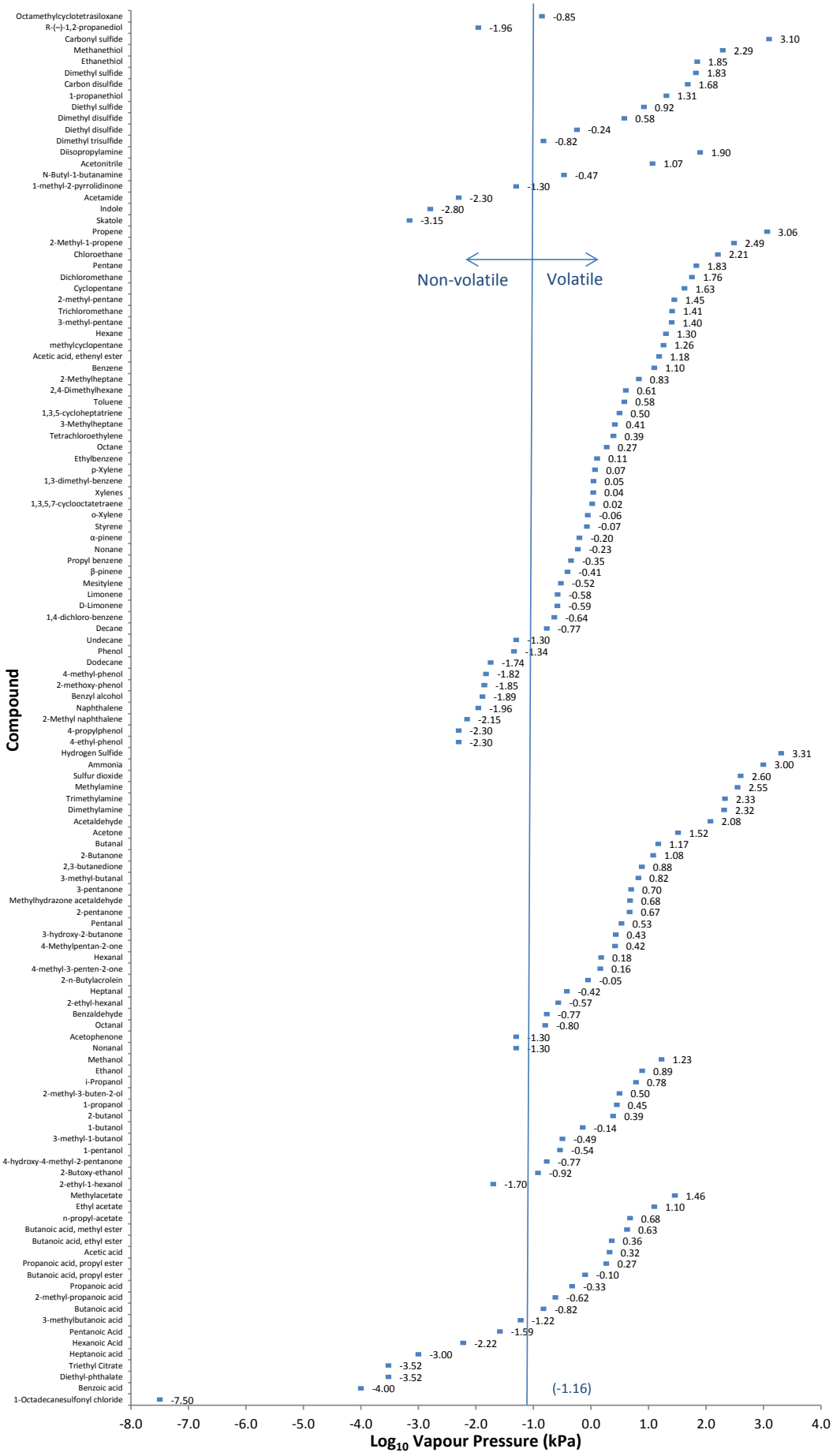


Figure S1.4. Graphical Summary of vapour pressure for selected compounds (Table S1). Classification for volatile/non-volatile compounds from Cai et al. (2006)



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"Odour emissions from poultry litter – A review litter properties, odour formation and odorant emissions from porous materials"
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Supporting Information S2 – Detailed discussion of odour measurement and odour threshold values

S2.1. Odour concentration

Odour concentration is measured using dynamic dilution olfactometry and a panel of qualified human odour assessors. Odour assessment is performed using standardized methods such as EN 13725 (European Committee for Standardization, 2003) or AS/NZS 4323.3-2001 (Standards Australia/Standards New Zealand, 2001). According to these Standards, odour assessors qualify if their detection threshold for a reference odorant, *n*-butanol, falls within a specified range. Odour concentration is measured using odour units (ou). One odour unit is determined using a gas mixture containing 132 µg of n-butanol evaporated into one cubic metre of air at standard conditions (0 °C and 101.325 kPa), which is approximately equivalent to 40 ppbV. One odour unit is defined when this concentration of the reference odorant elicits a physiological response (detection threshold) in 50% of the odour panel. Odour concentration of a sample is then defined by the number of dilutions required to elicit the same physiological response from the qualified panel.

S2.2. Odour intensity

Odour intensity "is the intensity of the sensation that is triggered by an odour stimulus" (Schulz et al., 2002) or may otherwise be referred to as "the perceived strength of an odour" (Lebrero et al., 2011). Intensity is measured using a seven point scale: 0=not detectable, 1=very weak, 2=weak, 3=distinct, 4=strong, 5=very strong, 6=extremely strong. A relationship exists between the concentration of an odour (measured by detection threshold) and its perceived intensity according to the Weber-Fechner or Steven's models (Misselbrook et al., 1993; Ouellette et al., 2010; Zhang et al., 2002). The Weber-Fechner model relates odour intensity to the $\log_{10}$ odour concentration whereas the Steven's model relates odour intensity to odour concentration using a power function (Zhang et al., 2002). As an example of what exponent may be required for meat chicken farm odours, Zhang et al. (2002) determined that an exponent of 0.57 was required to relate odour concentration to intensity for pig farm odour, although Misselbrook et al. (1993) found that meat chicken farm odours registered a higher intensity score for the same odour concentration compared to pig odours. Ouellette et al. (2010) referred to the exponent used in the Steven's model as 'the persistence' because it relates to how much an odour needs to be diluted to effect a change in the intensity. In practice, the $\log_{10}$ and power relationships between odour concentration and intensity mean that when the concentration of an odorant is near the odour threshold value, relatively small changes in odour concentration will result in a large change in perceived odour intensity while at much higher concentrations even large changes in the concentration of the odorant will result in small changes to perceived odour intensity.

S2.3. Odour descriptors

The third dimension used to describe an odour is odour quality, which provides a description of what an odour or individual odorant smells like. Odour wheels have developed to enable odour qualities/descriptions to be linked to specific odorants or groups of odorants (Decottignies et al., 2013; Suffet and Rosenfeld, 2007). Table S1 in the Supplementary Data lists reported odour qualities/descriptors for selected meat chicken odorants.

S2.4. Odour pleasantness

The fourth dimension used to describe an odour is hedonic tone, which uses a scale to rate the relative pleasantness or unpleasantness of odours (Lebrero et al., 2011; Nimmermark, 2011). The scale ranges from extremely unpleasant to extremely pleasant. One complication regarding hedonic tone is that some odours become less pleasant as the concentration of that odour increases (Nimmermark, 2011).

S2.5. Odour threshold values for individual odorants

Instrumental techniques provide information about the chemical composition of an odour but not the way that it is perceived by human receptors. Single compound odour thresholds (SCOT) (Parker et al., 2012), otherwise reported as an odour threshold (OT); odour threshold value (OTV); or odour detection threshold (ODT), have been determined so the contribution of individual odorants to likely odour impact/annoyance can be estimated. (Table S1 and Figure S1.1 in the Supplementary Data list odour threshold values for selected meat

chicken odorants). One way to conceptually estimate the relative contribution of an individual odorant to an odour mixture is to calculate its odour activity value (OAV), which is defined as the ratio of the airborne concentration of this compound to its odour threshold (Parker et al., 2013; Parker et al., 2012; Trabue et al., 2008). For complex odour mixtures, Capelli et al. (2013) explains that these individual odorant OAV values can be summed to provide an OAV for the mixture, presumably for comparison to other complex odour mixtures. OAV calculations can be imprecise due to difficulties in finding reliable odour threshold values and the values reported in the literature can vary by several orders of magnitude for individual odorants (Capelli et al., 2013; Parker et al., 2012). Ruth (1986) explained that some of the differences in reported OT values is related to the way odour threshold is defined. Some authors consider the OT value to be the lowest concentration at which one person can detect an odour while others consider the OT value to be the concentration at which 50–100% of a trained odour assessment panel can detect the odour (Hellman and Small, 1974; Ruth, 1986). Further complicating the use of OT and OAV is that the intensity to concentration relationship (as defined using the Weber-Fechner or Steven's models) is different for different compounds (Zhang et al., 2010). This means that even if two compounds/odour mixtures have a similar OAV, one may be perceived as having higher intensity.

The contribution of individual compounds to the perceived odour of an odour mixture in terms of intensity and character is very complex. Ruth (1986) explained that the odour threshold resulting from the mixture of two odorants can be independent ($OT_{AB} = OT_A$ or OT_B), additive ($OT_{AB} = OT_A + OT_B$), synergistic ($OT_{AB} > OT_A + OT_B$) or counteractive ($OT_{AB} < OT_A + OT_B$) compared to the thresholds of the individual odorants (where OT_{AB} is the odour threshold of the mixture of compounds A and B; OT_A is the odour threshold of compound A; and OT_B is the odour threshold of compound B). In contrast, calculations of OAV for individual compounds (Parker et al., 2013) or complex mixtures (Capelli et al., 2013) assume the relationship to be simply additive. Considering that odour from litter and meat chicken sheds is known to be a complex mixture of dozens of odorants it would seem unlikely that simple arithmetic would apply to the summation of odorant contributions to the whole odour mixture while assuming no interactions between the compounds.

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"Odour emissions from poultry litter – A review litter properties, odour formation and odorant emissions from porous materials"

Mark W. Dunlop, Patrick J. Blackall and Richard. M. Stuetz

Supporting Information S3

Table S3.1 Selected odorant producing bacterial genera and fungi reported to exist in meat chicken lower gastro-intestinal tract and litter (refer to footnotes for references)

Organism (Genus)	References (reported in meat chickens)		Description of preferred conditions	Odorants produced by organism
	Excreta or intestinal tract	Litter		
Atopostipes		17, 7	Facultative anaerobic conditions[7]	Organic acids; 3-hydroxy-2-butanone and dimethyl disulfide[16]
Bacillus	11, 2, 8, 18	1, 3, 17, 9	Min. water activity 0.93–0.95[13]	3-hydroxy-2-butanone and dimethyl disulfide[16]; 2-butanol, 2,3-butanedione, hexanone, methylallyl acetate, 2,6-dimethyl-3-heptanone[17]; sulfur compounds[19]; propylamine, iso-butylamine, amylamine, iso-amylamine, diaminoethane[12]; indole[6]
Bacteroides	11, 15, 2, 21, 14, 8, 18		pH 5–8.5[20]; 25–45 °C[20]; Anaerobic conditions[20]	Formic, acetic, propionic, butyric; iso-butyric, valeric, caproic, iso-valeric and iso-caproic acids; ammonia and volatile amines[20]; methyl-, ethyl-, propyl-, butyl-, amyl-, iso-butyl-, iso-amyl-, hexyl-, dipropyl- and dibutyl-amine[12]; amines, ammonia and indole[6]
Bifidobacterium	21, 8, 10			Amines and ammonia[6]
Brevibacterium	15	17, 7, 9		Dimethyl trisulfide[17]
Clostridium	11, 2, 10, 21, 14, 8, 18	1, 9	pH 6.5–7[20]; 15–69 °C[20]; Most strains do not tolerate oxygen[20]; Min. water activity 0.93–0.97[13]	Formic, acetic, propionic, butyric; iso-butyric, valeric, caproic, iso-valeric and iso-caproic acids; indoles and phenols[20]; 3-hydroxy-2-butanone and dimethyl disulfide[16]; dimethylamine, ethylamine, 1,4-diaminobutane[12]; skatole, indole and phenols[6]
Corynebacterium	15	17, 7, 9	Resistant to desiccation and starvation[7]; Anaerobic conditions [9]	Fatty acids, aldehydes, alcohols, volatile aliphatic acids (C_2-C_{11}), sulfur compounds[19]; methyl-, ethyl-, propyl-, butyl-, amyl-, iso-butyl-, iso-amyl-, hexyl-, dipropyl- and dibutyl-amine[12]
Desolfotomaculatum		9	Anaerobic conditions [9]	Reduced sulfates including Carbonyl sulfide, Carbon disulfide, methyl-mercaptan, ethyl-mercaptan and propyl-mercaptan[6]
Desolfovibrio	11		Anaerobic conditions[6]	Reduced sulfates including Carbonyl sulfide, Carbon disulfide, methyl-mercaptan, ethyl-mercaptan and propyl-mercaptan[6]
Enterococcus	11, 2, 8	9		2,3-Butanedione and 2,3-Butanediol[17]
Escherichia	11, 21, 14, 8	1, 3	Min. water activity 0.95[13]	Formic, acetic, propionic and butyric acids; indoles and phenols[20]; methyl-, ethyl-, propyl-, butyl-, amyl-, iso-butyl-, iso-amyl-, hexyl-, dipropyl- and dibutyl-amine[12]; indole and phenols[6]
Eubacterium	11, 2, 21, 8, 10, 18	7	pH 6.5–7.5[20]; 20–45 °C[20]; Anaerobic conditions[20]	Formic, acetic, propionic, butyric; iso-butyric, valeric, caproic, iso-valeric and iso-caproic acids; indoles and phenols[20]; methyl-, ethyl-, propyl-, butyl-, amyl-, iso-butyl-, iso-amyl-, hexyl-, dipropyl- and dibutyl-amine[12]
Faecalibacterium	11, 2, 14, 18		Some strains are obligate anaerobes[14]	Butyric acid and other short chain fatty acids[14]

Table S3.1 cont'd

Organism (Genus)	References (reported in meat chickens)		Description of preferred conditions	Odorants produced by organism
	Excreta or intestinal tract	Litter		
Fusobacterium	8			Indole[6]
Lactobacillus	11, 15, 21, 14, 8, 18	3, 17, 7, 9	Resistant to lower pH conditions[7]	Formic, acetic, propionic and butyric acids[20]; 2,3-Butanedione and 2,3-Butanediol[17]; 3-hydroxy-2-butanone and dimethyl disulfide[16]; skatole[6]
Leuconostoc	11			2,3-Butanedione and 2,3-Butanediol[17]
Megasphaera	15		pH 7.4–8.0[20]; 25–40 °C[20]; Anaerobic conditions[20]	Formic, acetic, propionic, butyric; iso-butyric, valeric, caproic, iso-valeric and iso-caproic acids; volatile sulfur containing compounds[20]
Peptostreptococcus	10		pH 6–8[20]; 25–45 °C[20]; Anaerobic conditions[20]	Formic, acetic, propionic, butyric; iso-butyric, valeric, caproic, iso-valeric and iso-caproic acids; ammonia and volatile amines[20]
Propionibacterium	21		pH 6.5–7.5[20]; 30–37 °C[20]; Anaerobic but tolerate oxygen[20]	Formic, acetic, propionic, butyric; iso-butyric, valeric, caproic, iso-valeric and iso-caproic acids; indoles and phenols[20]; fatty acids, aldehydes, alcohols[19]; indole[6]
Proteus	21			2,3-Butanedione, 3-hydroxy-2-butanone, 3-methyl-1-butanol, dimethyl disulfide[16]; methyl-, ethyl-, propyl-, butyl-, amyl-, iso-butyl-, iso-amyl-, hexyl-, dipropyl- and dibutyl-amine, 3-methylbutylamine, 2-phenylethylamine[12]; indole[6]
Pseudomonas	11, 21		Some species are capable of aerobic respiration[21]	methyl-, ethyl-, propyl-, butyl-, amyl-, iso-butyl-, iso-amyl-, hexyl-, dipropyl- and dibutyl-amine[12]
Salmonella	5, 11	1, 5	Min. water activity 0.92–0.95[13]	Hydrogen sulfide[5]
Shigella	11			Indole[6]
Staphylococcus		3, 17, 7, 9	Facultative anaerobe and tolerates dry and salty conditions[7]; Min. water activity 0.86[13]	Dimethyl disulfide, acetone[16]; fatty acids, aldehydes, alcohols[19]; sulfur compounds[19]; methyl-, ethyl-, propyl-, butyl-, amyl-, iso-butyl-, iso-amyl-, hexyl-, dipropyl- and dibutyl-amine[12]
Streptococcus	11, 8	3, 7	pH 4–9.6[20]; 15–45 °C[20]; Oxygen tolerant[20]; facultative anaerobe[7]	Formic, acetic, propionic and butyric acids; ammonia and volatile amines[20]; methyl-, ethyl-, propyl-, butyl-, amyl-, iso-butyl-, iso-amyl-, hexyl-, dipropyl- and dibutyl-amine[12]; amines[6]
Fungi				
Aspergillus		1, 17	Min. water activity 0.76–0.83[13]	1,10-dimethyl1,9-decanol; 3,octanone; nerodiol; 2-octen-1-ol; 1-octen-3-ol and phenylethyl alcohols[17]
Penicillium		17	Min. water activity 0.79–0.87[13]	1,10-dimethyl1,9-decanol; 3,octanone; nerodiol; 2-octen-1-ol; 1-octen-3-ol and phenylethyl alcohols[17]
Eurotium		17	Min. water activity 0.70-0.71[4]	1,10-dimethyl1,9-decanol; 3,octanone; nerodiol; 2-octen-1-ol; 1-octen-3-ol and phenylethyl alcohols[17]

[1]Bolan *et al.* (2010); [2]Choi *et al.* (2014); [3]Fries *et al.* (2005); [4]Fontana (2007); [5]Kizil *et al.* (2015); [6]Le *et al.* (2005); [7]Lovanh *et al.* (2007); [8]Lu *et al.* (2003a); [9]Lu *et al.* (2003b); [10]Mead (1989); [11]Singh *et al.* (2014); [12]Spoelstra (1980); [13]Taoukis and Richardson (2007); [14]Torok *et al.* (2011); [15]Videnska *et al.* (2014); [16]Wadud (2011); [17]Wadud *et al.* (2012); [18]Wei *et al.* (2013); [19]Wood and Kelly (2010); [20]Zhu *et al.* (1999); [21]Zhu *et al.* (2002)

Table S3.2 Extended list of bacterial genera reported to exist in meat chicken lower gastro-intestinal tract and litter but information regarding odorant production was not found (refer to footnotes for references)

Organism (Genus)	References (reported in meat chickens)		Description of preferred conditions
	Excreta or lower intestinal tract	Litter	
Achromobacter	8		
Acinetobacter	11	3, 17	
Aerococcus		3, 17, 9	
Alcaligenes	8	9	
Alistipes	11, 2, 14		
Anaerostipes	18		
Aquamicrobium		9	
Arthrobacter		1, 7, 9	Resistant to desiccation and starvation[7]
Blautia	11, 2, 18		
Bordetella		9	
Brachybacterium		17, 7, 9	
Butyrivibrio	18		
Campylobacter	8	1	Min. water activity 0.98[13]
Cellulomonas		9	
Citrobacter	11		
Denitrobacter		9	
Enterobacter	11		
Erysipelothrix	2		
Facklamia		17, 7, 9	
Flavobacterium	8	3	
Gallibacterium	14		
Gemmiger	10, 21		
Geobacter		9	
Georgenia		9	
Globicatella		9	Anaerobic conditions[9]
Hespellia	18		
Haemophillus	11		
Jeotgalicoccus		17, 7	
Klebsiella	11		
Listeria	11	1, 3	Min. water activity 0.92–0.94[13]
Lysobacter		9	
Megamonas	18		
Moraxella		3	
Nosocomilcoccus		17	
Ochrobacterium	8		
Oscillibacter	2		
Parabacteriodes	11, 18		
Paracoccus		9	
Pediococcus		3, 9	
Prevotella	11, 15		
Pseudoflavonifractor	11		
Roseburia	18		
Ruminococcus	11, 15, 21, 14, 8, 18	7, 9	
Salinicoccus		17, 7, 9	
Sphingobacterium		17, 9	
Stenotrophomonas		9	
Subdoligranulum	11, 2		
Tetragenococcus	2		
Trichococcus		17, 9	
Vagococcus		9	
Veillonella	11, 18		
Vibrio	11		Min. water activity 0.94[13]
Virgibacillus		17, 7	
Weisella	8		
Xanthomonas		9	
Yania		17	
Yersinia	11		Min. water activity 0.95[13]

[1]Bolan *et al.* (2010); [2]Choi *et al.* (2014); [3]Fries *et al.* (2005); [4]Fontana (2007); [5]Kizil *et al.* (2015); [6]Le *et al.* (2005); [7]Lovanh *et al.* (2007); [8]Lu *et al.* (2003a); [9]Lu *et al.* (2003b); [10]Mead (1989); [11]Singh *et al.* (2014); [12]Spoelstra (1980); [13]Taoukis and Richardson (2007); [14]Torok *et al.* (2011); [15]Videnska *et al.* (2014); [16]Wadud (2011); [17]Wadud *et al.* (2012); [18]Wei *et al.* (2013); [19]Wood and Kelly (2010); [20]Zhu *et al.* (1999); [21]Zhu *et al.* (2002)

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"Odour emissions from poultry litter – A review litter properties, odour formation and odorant emissions from porous materials"
by Mark W. Dunlop, Patrick J. Blackall and Richard. M. Stuetz

Supporting Information S4 – Detailed discussion of the diffusion and emission of odorants from porous media

S4.1. Molecular diffusion and boundary theories

Diffusion and transport of gases from liquid and porous media are complex and dynamic processes that have previously been described or reviewed by Capelli et al. (2012), Hudson and Ayoko (2008), Jähne and Haußecker (1998), Parker et al. (2010), Schwarzenbach et al. (2003), Thibodeaux and Scott (1985) and Zhang et al. (2002). Molecules of a compound move randomly within a medium (e.g. air) and collide with other molecules. The behaviour and movement of molecules within the medium is governed by the ability of the molecule to move within the medium. This is described in terms of molecular diffusivity and quantified using a diffusion coefficient (Schwarzenbach et al., 2003). If there is a concentration gradient of the compound in the medium, the compound will diffuse from the place of high concentration to low concentration at a rate proportional to the gradient. *Fick's Law* is used to describe the steady state diffusive flux of the compound by incorporating its diffusion coefficient and the concentration gradient (Schwarzenbach et al., 2003; Thibodeaux and Scott, 1985).

Molecules of a compound will eventually reach the boundary of the medium through which they are diffusing. When they reach the boundary, additional forces will act on the molecules, affecting the rate at which the molecules can travel through the boundary (i.e. provide resistance). Boundaries are considered to be any change in the properties of the medium or boundary/interface of a new medium. The following are some examples:

- changes in temperature (e.g. thermoclines)
- changes in phase (i.e. solid to liquid, solid to gas, liquid to gas and vice-versa)
- changes in density (e.g. compaction of a solid or porous material)
- changes in material (e.g. water to air, film/cover on a liquid surface)
- change in chemical concentration/compound
- change in turbulence.

In the case of poultry litter, the boundary may be the surface of the litter/cake, the surface of individual litter particles, or the surface of a film of moisture surrounding individual litter particles.

Theories on diffusion and boundary transfer are applied to the emission of volatile compounds from liquids, solid and/or porous materials (Schwarzenbach et al., 2003; Thibodeaux and Scott, 1985). One common feature of these models is the assumption that there is resistance preventing the flux of volatile compounds from the source into the airstream and vice-versa. This resistance is commonly viewed as layers. A layer exists in the air phase and is referred to as a boundary layer while the layer in the source is referred to as a surface or sub-surface layer (Schwarzenbach et al., 2003).

Schwarzenbach et al. (2003) described three types of boundary, each identifiable by changes in diffusion rate on each side of the boundary or through the boundary:

1. *Bottleneck boundary*—characterised by an abrupt drop in diffusivity at the boundary when the zones on either side of the boundary have relatively unrestricted diffusivity. Classic examples of bottleneck boundaries are water-air interface, where molecules are relatively free to diffuse within each of the water and air zones, but the movement of molecules between the zones is restrictive.

   In the case of water-air interface there are multiple layers to the bottleneck boundary (there will likely be multiple layers at the boundary between any two different media). There is a layer at the boundary of the water (liquid phase boundary layer) and also at the boundary of the air (gas phase boundary layer). Each of these layers can independently influence the diffusivity of molecules through the water-air interface.

   Due to the requirement for unrestricted availability of molecules at the boundary, bottleneck boundaries will commonly have mixing/turbulence in the zones on each side of the boundary.

2. *Wall boundary* —characterised by a sudden change in diffusivity from one side of the boundary to the other (diffusivity changes by orders of magnitude). Zones on each side of the boundary may be the same media (e.g. a compacted layer) or different media (e.g. water column on top of a sediment layer in a river).

3. *Diffusive boundary*—characterised by similar diffusion rates in both zones on each side of the boundary, but reduced rate of diffusion within the boundary. This can occur due to a change in physical property of a single medium (i.e. change in chemical concentration or temperature) or between two media that have similar diffusivity for the compound of interest.

It is suggested that emissions from meat chicken litter may be described using different boundary types depending on physical litter conditions. Surface and boundary layers exist on the overall litter surface and also on each particle within the litter. Dry, friable litter or cake may be described as a 'diffusive boundary' or 'wall boundary' depending on the amount of resistance to diffusion within the litter compared to the air above it. However, if a layer of cake is present on the litter surface, and the focus is emission of odorants from the base of the litter through the cake, then a 'bottleneck boundary' may be more appropriate (Fig. 2 in the main article).

Resistance to flux of a volatile compound can occur in either the air boundary layer or surface layer or both, depending on the specific compound, properties of the source (e.g. turbulence of a liquid or porosity and compaction of a solid) and conditions of the airflow above the surface. Convective mass transfer through the air boundary layer above the litter is affected by the thickness and conditions within the boundary layer (Capelli et al., 2012; Thibodeaux and Scott, 1985; Zhang et al., 2002). Increasing velocity and turbulence of air (as indicated by greater Reynolds number) break down the boundary layer and increase the mass convection of compounds from litter. Litter surface roughness also affects the boundary layer. Zhang et al. (2002) found that the surface roughness of soil (which we suggest is likely to be similar to litter) was sufficient to make the air boundary layer turbulent, thus avoiding laminar flow conditions.

It is a common assumption that gases move from a solid/porous/liquid source into the gas phase above it due to the much higher concentration of compounds in the source; however, the movement of compounds can theoretically be in both directions. Changes of concentration with the air or source; changes to physical conditions (e.g. changes in temperature); changes to the boundary layers; properties of the specific compound; and environmental conditions can trigger the change in direction of diffusion. Schwarzenbach et al. (2003) provided examples of how a change in temperature reverses the direction of flux for individual compounds due to changes in solubility and diffusivity of a particular compound in two different media, which occur due to changes in temperature. It may be unlikely that this reversal would occur during normal conditions in a meat chicken shed due to much higher concentration of odorant compounds within litter compared to the relatively low concentration of air above the litter; however, it may be a consideration with particular area-source sampling enclosures (e.g. flux hoods) that increase the concentration of compounds in the air above the litter to a condition that is closer to equilibrium. In this situation, changes in litter or ambient conditions may be sufficient to reverse the direction of odorant transport.

The 'two-film theory' — also be known as the 'stagnant-film model' (Parker et al., 2010) — is one boundary layer theory that has previously been used to explain the transfer of gases between the liquid and gas phase (Hudson and Ayoko, 2008; Parker et al., 2010). The two film theory is applicable to quiescent (still) water bodies and still air conditions at the boundary between the liquid and gas phases. Litter is not a quiescent water body and therefore the two film theory may have limited applicability for modelling odorant emissions due to litter conditions and ventilation practices. It is suggested that this theory may be applicable when litter has moderate to high litter moisture content because moisture will surround litter particles and fill pores within the litter.

S4.2. Henry's Law

Integral with the two-film theory is Henry's Law, which was defined by Parker et al. (2010) as follows: "that at equilibrium, the VOC concentration in the air is directly proportional to the VOC concentration in the water". Henry's Law constants enable the definition of a steady state ratio in the concentration of a compound in the liquid phase to the concentration of the specific compound in the gas phase above it. Each compound has a different Henry's law constant and will therefore reach equilibrium with different conditions in both the liquid and gas phase. Henry's law constants also provide a guide for which conditions, turbulence and/or phenomena control the emission (Hudson and Ayoko, 2008; Parker et al., 2010; Schwarzenbach et al., 2003).

To add a complication, Henry's law constants may be presented using one of four different units, some with dimensions and some dimensionless (Staudinger and Roberts, 1996). Additionally, the value of a Henry's law constant assigned to a compound changes with temperature (published values are usually quoted at either 20 °C or 25 °C), pH, compound hydration, compound concentration as well as the presence of other compounds, dissolved salts, dissolved organic matter and suspended solids (due to adsorption of compounds onto the solids surfaces) (Staudinger and Roberts, 1996). Consequently published values should be considered as approximate only (Hudson and Ayoko, 2008).

When using Henry's law constants to explain emissions, the dimensionless values (or $\log_{10}$ of the dimensionless value) is common (Hudson and Ayoko, 2008; Parker et al., 2010; Schwarzenbach et al., 2003; Staudinger and Roberts, 1996, 2001) although some of the largest compilations of Henry's law constants tend to use dimensional values (NIST, 2013; Sander, 1999). Henry's law constants for selected meat chicken shed odorants are provided in Table S1 and Figure S1.3 in the Supporting Data. The Henry's law constant assigned to each compound can be used as an indication of the relative importance of ventilation air speed/turbulence or litter moisture content on odorant emissions from litter.

Emissions of compounds with a dimensionless Henry's law constant value less than 1.0×10^{-3} are driven by physical phenomena in the gas phase (i.e. in-shed ventilation air speed and turbulence), while compounds with a Henry's law constant value greater than 1.0×10^{-3} are driven by physical phenomena within the liquid (Hudson and Ayoko, 2008; Parker et al., 2010). Hudson and Ayoko (2008) further categorised the compounds into three categories: emission rates for compounds with dimensionless Henry's law constant less than $1.0 \times 10^{-3.3}$ are gas phase controlled; emission rate for compound with dimensionless Henry's law constant between $1.0 \times 10^{-3.3}$ and $1.0 \times 10^{-1.3}$ are both gas and liquid phase controlled; while the emission rates for compounds with Henry's law constant greater than $1.0 \times 10^{-1.3}$ are liquid phase controlled.

The two-film theory is traditionally applied to quiescent water bodies rather than moist porous materials such as meat chicken litter or meat chicken litter cake. With porous materials, fluxes of VOCs and water are reduced by internal resistance and by some molecules of the compound being adsorbed on particle surfaces (Ghaly and MacDonald, 2012; Schwarzenbach et al., 2003; Staudinger and Roberts, 1996; Yusheng and Poulsen, 1988; Zhang et al., 2002). Internal resistance and diffusion from litter are affected by:

- cake (thickness, moisture content and density);
- porosity (affected by particle size, compaction, moisture content, faeces content);
- moisture content (affecting the availability of water for evaporation); and
- air conditions above the litter (temperature, humidity and concentration of compounds being emitted that are already in the air).

Evaporation of water has been found to be representative of the emission of gas-phase controlled odorants, which includes many of the odorants identified as contributing to odour impacts (Parker et al., 2013a; Parker et al., 2010; Parker et al., 2013b). The advantage of using water evaporation (water flux) instead of odorants is the relative ease, low cost and accuracy of measuring water evaporation using a readily available laboratory balance. Further experimental work is required to quantify the effects of temperature, humidity, litter porosity (cake compared to friable litter), litter pH, air speed and other factors on evaporation of water from meat chicken litter so this flux can be related to emission of gas-phase controlled odorants.

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