

Table S1 – classification of VOCs according to disease states and sample source

Disease	Sample source	Chemical family	VOC	CAS number	Ref
Allograft rejection	Breath	Organosulphur	Carbonyl sulfide	463-58-1	[1]
Alzheimer	Breath	Acid	2,2-dimethyl-propanoic acid	75-98-9	[2]
			Oxalic acid	144-62-7	[2]
		Alcohol	2,6-octadien-1-ol	N/A	[2]
			2-butyl-1-octanol	3913-02-8	[2]
		Alkane	1-chloro-nonadecane	62016-76-6	[2]
			1-methylpropyl-cyclooctane	16538-89-9	[2]
			2,3,5-trimethylhexane	1069-53-0	[2]
			2,3-dimethyl-heptane	3074-71-3	[2]
			2,5,6-trimethyl-octane	62016-14-2	[2]
			2,6,10- trimethyl-dodecane	3891-98-3	[2]
			2,6,10,14-tetramethyl-hexadecane	638-36-8	[2]
			3,7-dimethyl-decane	17312-54-8	[2]
			3-ethyl-2,2-dimethyl-pentane	16747-32-3	[2]
			4-methyl-octane	2216-34-4	[2]
			5-ethyl-2-methyl-octane	62016-18-6	[2]
			Dodecane	112-40-3	[2]
			Heptane ,2,2,4,6,6-pentamethyl-	13475-82-6	[2]
		Alkene	2,4-dimethyl-1-heptene	19549-87-2	[2]
		Aromatic	1-methylethyl-benzene	N/A	[2]
			Butylated hydroxytoluene	128-37-0	[2]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			Propyl benzene	103-65-1	[2]
			Styrene	100-42-5	[2]
		Ester	2-ethylhexyl tetradecyl ester	N/A	[2]
			1,1'-oxybis-octane (octyl ether)	629-82-3	[2]
		Other	3,7-dimethyl-propanoate	144-39-8	[2]
Asthma	Breath	Alkane	Ethane	74-84-0	[3]
			Pentane	109-66-0	[4]
		Amine	Ammonia	7664-41-7	[5, 6]
		Nitrile	NO	10102-43-9	[7, 8]
		Other	8-isoprostane	27415-26-5	[9]
			Hydrogen peroxide	7722-84-1	[10]
Breast cancer	Breath	Alcohol	2-hexyl-1-octanol	19780-79-1	[11]
		Alkane	2,3,4-trimethyldecane	62238-15-7	[12]
			3,3-dimethyl pentane	562-49-2	[12]
			5-(2-methylpropyl)nonane	62185-53-9	[12]
			Dodecane, 4-methyl	6117-97-1	[13]
			Nonadecane, 3-methyl	6418-45-7	[13]
			Nonane	111-84-2	[13]
			Octane, 2-methyl	3221-61-2	[13]
			Pentadecane, 6-methyl	10105-38-1	[13]
			Propane, 2-methyl	75-28-5	[13]
			Tridecane	629-50-5	[11]
		Tridecane, 5-methyl	25117-31-1	[13]	
		Alkane	Undecane, 3-methyl	1002-43-3	[13]
		Aromatic	Benzene, 1,2,4,5-tetramethyl-	95-93-2	[11]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
		Nitrile	2-amino-5-isopropyl-8-methyl-1-azulenecarbonitrile	93946-48-6	[12]
		Other	(+)-Longifolene	475-20-7	[11]
			2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	719-22-2	[11]
			6-ethyl-3-octyl ester 2-trifluoromethyl benzoic acid	N/A	[12]
			Cyclopropane, ethylidene	18631-83-9	[11]
		Terpene	D-limonene	1461-27-4	[11]
Chronic renal failure/uremia	Breath	Alkane	2,2,6,6-tetramethyl-octane	62199-20-6	[14, 15]
			2,4-dimethyl heptane	2213-23-2]14 ,15[
		Amine	Ammonia	7664-41-7	[14, 15]
			Dimethyl amine	124-40-3	[14, 15]
			Trimethyl amine	75-50-3	[14, 15]
		Ketone	2-butanone	78-93-3	[14, 15]
Colorectal cancer	Breath	Aldehyde	Decanal	112-31-2	[16]
			Nonanal	124-19-6	[16]
		Alkane	1-iodo nonane	4282-42-2	[12]
			2-Methylbutane	78-78-4	[16]
			2-methyl-pentane	107-83-5	[16]
			3-Methylpentane	96-14-0	[16]
			4-methyl-octane	2216-34-4	[16]
			Cyclohexane	110-82-7	[16]
			Methylcyclohexane	108-87-2	[16]
		Alkane	Methyl-cyclopentane	96-37-7	[16]
1,2-Pentadiene	591-95-7		[16]		

Disease	Sample source	Chemical family	VOC	CAS number	Ref
		Aromatic	1,1'-(1-butenylidene)bis benzene	N/A	[12]
			1,3-Dimethylbenzene (m-Xylene)	108-38-3	[12] [16]
			P-xylene	106-42-3	[16]
		Ketone	4-Methyl-2-pentanone	1108-10-1	[16]
		Nitrile	2-amino-5-isopropyl-8-methyl-1-azulenecarbonitrile	93946-48-6	[12]
		Organosulphur	[(1,1-dimethylethyl)thio] acetic acid	N/A	[12]
		Other	4-(4-propylcyclohexyl)-, 4'-cyano[1,1'-biphenyl]-4-yl ester benzoic acid	N/A	[12]
COPD	Breath	Aldehyde	Heptanal	111-71-7	[17]
			Hexanal	66-25-1	[17, 18]
			Malondialdehyde	N/A	[17]
			Nonanal	124-19-6	[17]
		Alkane	2,4,6-Trimethyl-decane	N/A	[18]
			2,6-dimethyl-heptane	N/A	[18]
			4,7dimethyl-undecane	17301-32-5	[18]
			4-methyl-octane	2216-34-4	[18]
			Ethane	74-84-0	[19]
			Hexadecane	544-76-3	[18]
			Octadecane	N/A	[18]
			Undecane	1120-21-4	[18]
		Alkene	Isoprene	78-79-5	[18]
		Nitrile	Benzonitrile	N/A	[18]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			NO	10102-43-9	[20]
		Other	3,7-Dimethyl 1,3,6-octatriene	N/A	[18]
			Hydrogen peroxide	7722-84-1	[21]
			Terpineol	8000-41-7	[18]
Cystic fibrosis	Breath	Nitrile	NO	10102-43-9	[22, 23]
		Organosulphur	Carbonyl sulfide	463-58-1	[24]
Diabetes mellitus	Breath	Alcohol	Ethanol	64-17-5	[25]
		Ester	Methyl nitrate	598-58-3	[26]
		Ketone	Acetone	67-64-1	[25]
Gastric Cancer	Breath	Aldehyde	Furfural	98-01-1	[27, 28]
		Alkane	4,5-dimethyl-nonane	N/A	[27]
			4-methyl-octane	2216-34-4	[28]
			Hexadecane	544-76-3	[28]
		Alkene	Isoprene	78-79-5	[27]
		Aromatic	1,2,3-trimethyl-benzene	526-73-8	[28]
			A-methyl-styrene	98-83-9	[28]
		Ester	2-pentyl acetate	626-38-0	[27]
			2-butoxy-ethanol	111-76-2	[27, 28]
		Ketone	2-butanone	78-93-3	[28]
6-methyl-5-hepten-2-one	110-93-0		[27]		
Other	Acrylnitril	107-13-1	[27, 28]		
Gastrointestinal disease	Breath	Acid	Acetic acid	64-19-7	[29]
			Hexanoic acid	142-62-1	[29]
			Pentanoic acid	109-52-4	[29]
		Alcohol	1-pentanol	71-41-0	[29]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			1-propanol	71-23-8	[29]
			Butanol	71-36-3	[29]
			Ethanol	64-17-5	[30]
			Methanol	67-56-1	[29]
		Aldehyde	Butanal	1123-72-8	[29]
			Decanal	112-31-2	[29]
			Heptanal	111-71-7	[29]
			Hexanal	66-25-1	[29]
			Nonanal	124-19-6	[29]
			Octanal	124-13-0	[29]
			Pentanal	110-62-3	[29]
			Propanal	123-38-6	[29]
		Alkane	3-methyl-hexane	589-34-4	[30]
			5-ethyl-2-methyl-octane	62016-18-6	[30]
			Dodecane	112-40-3	[30]
			Ethane	74-84-0	[31]
			Pentane	109-66-0	[31, 32]
			Propane	74-98-6	[31]
		Alkene	2,4-dimethyl-1-heptene	19549-87-2	[30]
			Isoprene	78-79-5	[29]
			Tetrachloroethylene	N/A	[30]
		Amine	Ammonia	7664-41-7	[29]
		Aromatic	Ethyl phenol	123-07-9	[29]
Phenol	108-95-2		[29]		

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			Phenol, 4-methyl	106-44-5	[29]
		Ketone	2-butanone	78-93-3	[30]
			Acetone	67-64-1	[29]
		Nitrile	Hydrogen cyanide	74-90-8	[29]
		Organosulphur	Carbon disulfide	75-15-0	[29]
			Dimethyl disulphide	624-92-0	[29]
			Dimethyl sulphide	75-18-3	[29]
			Hydrogen sulfide	7783-06-4	[29]
		Feces	Acid	Acetic acid	64-19-7
	Pentanoic acid, 4-methyl			N/A	[33]
	Alcohol		1-Propanol, 2-methyl	78-83-1	[33]
			2-Butanol	78-92-2	[33]
			Methanol	67-56-1	[33]
	Aldehyde		Heptanal	111-71-7	[33]
			Pentanal	110-62-3	[33]
			Propanal	123-38-6	[33]
	Alkane		Undecane	1120-21-4	[33]
	Amine		Ammonia	7664-41-7	[34]
	Aromatic		1-Methyl-2-(1-methylethyl)-benzene (o-Cymene)	527-84-4	[33]
			1-methyl-3-(1-methylethyl)-benzene (m-Cymene)	535-77-3	[33]
			Ethylbenzene	100-41-4	[33]
			Indole	120-72-9	[34]
		Phenol	108-95-2	[34]	
Phenol, 4-methyl		106-44-5	[33]		

Disease	Sample source	Chemical family	VOC	CAS number	Ref
		Ester	Acetic acid, pentyl ester	N/A	[33]
			Benzoic acid, 2-hydroxy-, methyl ester	N/A	[33]
			Butanoic acid, 2-methyl-, propyl ester	N/A	[33]
			Butanoic acid, 2-methylbutyl ester	N/A	[33]
			Butanoic acid, 2-methylpropyl ester	N/A	[33]
			Butanoic acid, 3-methyl-, butyl ester	N/A	[33]
			Butanoic acid, 3-methyl-, methyl ester	N/A	[33]
			Butanoic acid, 3-methyl-, propyl ester	N/A	[33]
			Butanoic acid, 3-methyl-methyl ester	N/A	[33]
			Butanoic acid, butyl ester	N/A	[33]
			Butanoic acid, ethyl ester	N/A	[33]
			Butanoic acid, methyl ester	N/A	[33]
			Butanoic acid, propyl ester	N/A	[33]
			Cyclohexanecarboxylic acid, butyl ester	N/A	[33]
			Cyclohexanecarboxylic acid, ethyl ester	N/A	[33]
			Cyclohexanecarboxylic acid, methyl ester	N/A	[33]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			Cyclohexanecarboxylic acid, propyl ester	N/A	[33]
			Ethanoic acid, 3-methyl-1-butyl ester	N/A	[33]
			Ethanoic acid, ethyl ester	N/A	[33]
			Hexanoic acid, methyl ester	N/A	[33]
			Pentanoic acid, 4-methyl-, pentyl ester	N/A	[33]
			Pentanoic acid, butyl ester	N/A	[33]
			Pentanoic acid, methyl ester	N/A	[33]
			Propanoic acid, 2-methyl-, methyl ester	N/A	[33]
			Propanoic acid, 2-methylpropyl ester	N/A	[33]
			Propanoic acid, 3-methyl-1-butyl ester	N/A	[33]
			Propanoic acid, butyl ester	N/A	[33]
			Propanoic acid, methyl ester	N/A	[33]
			Propanoic acid, propyl ester	106-36-5	[33]
		Ketone	2-Heptanone, 6-methyl	928-68-7	[33]
			2-Piperidinone	675-20-7	[33]
			5-Methyl-2-(1-methylethyl)-cyclohexanone	10458-14-7	[33]
			6-methyl-5-hepten-2-one	110-93-0	[33]
		Organosulphur	S-Methyl 3-methylbutanethioate	23747-45-7	[33]
			Thiopicvalic acid	55561-02-9	[33]
		Other	1-Butanol, 3-methyl-,	105-68-0	[33]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			propanoate		
			4-Methyl-1-Indole	N/A	[33]
			5-methyl-2-(1-methylethyl)-cyclohexanol	15356-70-4	[33]
			A'-Phellandrene	99-83-2	[33]
			Copaene	3856-25-5	[33]
			Methoxy-phenyl-oxime	N/A	[33]
		Terpene	A'-Pinene	80-56-8	[33]
			γ-terpinene	99-85-4	[33]
Halitosis	Breath	Acid	Butyric acid	107-92-6	[35]
		Amine	Ammonia	7664-41-7	[35]
			Dimethyl amine	124-40-3	[35]
			Trimethyl amine	75-50-3	[35]
		Aromatic	Skatole	83-34-1	[35]
		Organosulphur	Allyl mercaptan	870-23-5	[35]
			Allyl methyl sulfide	10152-76-8	[35]
			Carbon disulfide	75-15-0	[35]
			Dimethyl sulphide	75-18-3	[35]
			Ethyl-propyl-sulfide	4110-50-3	[35]
	Hydrogen sulfide		7783-06-4	[36]	
	Methyl mercaptan		74-93-1	[36]	
	Propyl-mercaptan	107-03-9	[35]		
Saliva	Organosulphur	Hydrogen sulfide	7783-06-4	[37]	
		Methyl mercaptan	74-93-1	[37]	
Head and neck cancer	Breath	Acid	2,2-dimethyl-propanoic acid	75-98-9	[38]
		Alkane	2,2-dimethyl-decane	17302-37-3	[38]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			2,4-dimethyl heptane	2213-23-2	[38]
			4,6-Dimethyl-dodecane	61141-72-8	[38]
		Ketone	5-methyl-3-hexanone	623-56-3	[38]
		Other	2,2,3-erimethyl-, exobicyclo[2.2.1]heptane	N/A	[38]
		Terpene	Limonene	138-86-3	[38]
Heart allograft rejection	Breath	Alkane	Breath Alkanes	N/A	[39]
Heat failure	Breath	Nitrile	NO	10102-43-9	[40]
Hepatic cancer/cirrhosis	Blood	Aldehyde	Hexanal	66-25-1	[41]
		Alkane	1-octen-3-ol	3391-86-4	[41]
		Alkane	Octane	111-65-9	[41]
		Alcohol	3-Methylbutanol	123-51-3	[42]
	Breath	Acid	Propanoic acid	79-09-4	[43]
		Alcohol	1-Hexadecanol	36653-82-4	[43]
			Isopropyl alcohol	67-63-0	[43]
		Aldehyde	Acetaldehyde	75-07-0	[44, 45]
		Alkane	Octane	111-65-9	[43]
		Ketone	2-pentanone	107-87-9	[46]
			Acetone	67-64-1	[46]
		Organosulphur	Carbonyl sulfide	463-58-1	[44, 45]
			Dimethyl sulphide	75-18-3	[44, 45]
			Methyl mercaptan	74-93-1	[44, 45]
	Volatile sulphur containing compounds		N/A	[46-49]	
In vitro	Acid	Acetic acid	64-19-7	[50]	

Disease	Sample source	Chemical family	VOC	CAS number	Ref
		Alcohol	Ethanol	64-17-5	[50]
		Alkane	Octane	111-65-9	[50]
		Aromatic	2,3-di-hydro-benzofuran	496-16-2	[50]
		Organosulphur	Methane-sulfonyl chloride	124-63-0	[50]
Hyperglycemia	Breath	Aromatic	Ethylbenzene	100-41-4	[51]
			P-xylene	106-42-3	[51]
Kidney failure	Breath	Alkene	Isoprene	78-79-5	[52]
Kidney injury	Breath	Alcohol	Ethanol	64-17-5	[53]
		Ketone	2-pentanone	107-87-9	[53]
			Acetone	67-64-1	[53]
Lung cancer	Breath	Alcohol	4-penten-2-ol	625-31-0	[54]
			Ethanol	64-17-5	[55-57]
			Methanol	67-56-1	[58]
		Aldehyde	Butanal	1123-72-8	[59, 60]
			Formaldehyde	50-00-0	[61, 62]
			Heptanal	111-71-7	[59, 63-65]
			Hexanal	66-25-1	[57, 59, 63-65]
			Nonanal	124-19-6	[59, 62]
			Octanal	124-13-0	[62, 66, 67]
			Pentanal	110-62-3	[59, 62]
		Propanal	123-38-6	[59, 60]	
		Alkane	1,1,2-trichloro-1,2,2-trifluoro-ethane	N/A	[54]
			1-methyl-2-pentyl-cyclopropane	41977-37-1	[64]
2,3,4-trimethylhexane	921-47-1		[12]		

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			2,4-dimethyl heptane	2213-23-2	[64]
			2-methylheptane	592-27-8	[64]
			2-methylhexane	591-76-4	[13]
			2-methyl-pentane	107-83-5	[68]
			3,3-dimethyl pentane	562-49-2	[12]
			3-methyl-hexane	589-34-4	[13]
			3-methyl-nonane	599-04-6	[64]
			3-methyl-octane	3221-61-2	[64, 68]
			3-methyltridecane	6418-41-3	[13]
			4-methyl-octane	2216-34-4	[13]
			5-methyl-decane	17312-74-2	[13]
			7-methyl-tridecane	26730-14-3	[13]
			Butane	106-97-8	[55, 69, 70]
			Cyclohexane	110-82-7	[57, 64, 70, 71]
			Decane	124-18-5	[64, 68]
			Decane, 4-methyl	2847-72-5	[72]
			Dodecane	112-40-3	[12]
			Heptane	142-82-5	[63, 68, 69]
			Heptane ,2,2,4,6,6-pentamethyl-	13475-82-6	[64]
			Methyl-cyclopentane	96-37-7	[54, 64]
			Methylcyclopropane	594-11-6	[73]
			Octane	111-65-9	[56, 63]
			Pentane	109-66-0	[63, 68-70]
			Trichlorofluoro-methane	N/A	[64]
			Undecane	1120-21-4	[63, 64, 74, 75]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
		Alkene	1,3-butadiene,2-methyl-isoprene	N/A	[64]
			1,5,9-trimethyl-1,5,9-cyclododecatriene	21064-19-7	[72]
			1-heptene	592-76-7	[64, 68, 69]
			1-hexene	592-41-6	[73]
			2,3-hexadiene	592-49-4	[54]
			5,5-dimethyl-1,3-hexadiene	1515-79-3	[54]
			Isoprene	78-79-5	[55, 57, 63, 68, 74]
		Aromatic	1,1-(1,2-cyclobutanediyl)bis-,cis-benzene	7694-30-6	[54]
			1,1'-(1-butenylidene)bis benzene	N/A	[12] [54]
			1,2,3,4-tetrahydro-9-propyl-anthracene	N/A	[54]
			1,2,4,5-3,3,6,6-tetraphenyl-tetroxane	1073-91-2	[54]
			1,2,4-trimethyl benzene	95-63-6	[64, 68]
			1,4-dimethylbenzene (p-xylene)	106-42-3	[64]
			10,11-dihydro-5H-dibenzo-(B,F)-azepin	494-19-9	[72]
			1-methyl-4-(1-methylethyl)-benzene (p-Cymene)	99-87-6	[12]
			1-oxybis-benzene	N/A	[72]
			2,2-diethyl-1,1-biphenyl	605-39-0	[72]
			2,3-dihydro-1,1,3-trimethyl-3-phenyl-1-H-indene	3910-35-8	[72, 76]
			2,5-dimethyl furan	625-86-5	[60, 72, 76]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			2-ethyl-9,10-anthracenediol	N/A	[54]
			Aniline	62-53-3	[54]
			Benzene	71-43-2	[55, 63, 64, 68, 70, 74, 75]
			Benzophenone	119-61-9	[54]
			Diethylbenzene-1,2-dicarboxylate	84-66-2	[72]
			Ethyl-4-ethoxybenzoate	23676-09-7	[72, 76]
			Ethylbenzene	100-41-4	[58]
			O-toluidine	95-53-4	[54, 61]
			Propyl benzene	103-65-1	[63, 64, 75]
			Styrene	100-42-5	[64, 68, 70, 75]
			Toluene	108-88-3	[12, 68]
		Ester	2,2,4-trimethyl-pentan-1,3-dioldiisobutyrate	25265-77-4	[72]
			Propanoicacid,2,2,4-trimethyl-3-carboxyisopropyl,isobutylester	N/A	[54]
			2-methoxy-2-methyl-propane	1634-04-4	[54]
		Ketone	2,4-dimethyl-3-pentanone	565-80-0	[72]
			2,5-dimethyl-2,4-hexanedione	N/A	[72]
			2-butanone	78-93-3	[74]
			2-methyl-3-hexanone	N/A	[54]
			3-hydroxy-2-butanone (Acetoin)	513-86-0	[74, 77, 78]
			Acetone	67-64-1	[57, 63, 70, 74]
			A-isomethyl ionone	127-51-5	[54]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
		Nitrile	Acetonitrile	75-05-8	[60]
		Organosulphur	1-(methylthio)-(E)-1-propene	N/A	[54]
			1,1-[1-(ethylthio)propylidene]bis-benzene	N/A	[54]
			Carbon disulfide	75-15-0	[13]
			Dimethyl sulphide	75-18-3	[58]
		Other	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	N/A	[54]
			2,2,7,7-tetramethyltricyclo[6.2.1.0(1,6)]undec-4-en-3-one	N/A	[54]
			2,5-2,6-bis(1,1-dimethylethyl)-cyclohexadiene-1,4-dione	N/A	[72]
			2,6-bis(1,1-dimethylethyl)-4-ethylidene-2,5-cyclohexadien-1-one	N/A	[54]
			2-methyl-,1-(1,1-diamethylethyl)-2-methyl-1,3-propanediyl ester	N/A	[72, 76]
			5-(Ethoxycarbonyl)bicyclo[3.2.2]nonane-1-carboxylic acid	N/A	[54]
			5-isopropenyl-2-methyl-7-oxabicyclo[4.1.0]heptan-2-ol	N/A	[54]
			7,7-trimethyl-(1S)-bicyclo[2.2.1]heptan-2-one	N/A	[54]
			Camphor	76-22-2	[54]
			P-menth-1-en-8-ol (alpha-	98-55-5	[54]

Disease	Sample source	Chemical family	VOC	CAS number	Ref	
			Terpineol)			
			Trans-caryophyllene	N/A	[64]	
			A, α -4-trimethyl-3-cyclohexene-1-methanol	N/A	[54]	
	In vitro	Alcohol		2-ethyl-1-hexanol	104-76-7	[79]
		Aldehyde		3-methylbutanal	590-86-3	[66, 80, 81]
				Acetaldehyde	75-07-0	[66, 81-83]
				Butanal	1123-72-8	[84]
				Heptanal	111-71-7	[84]
				Hexanal	66-25-1	[80, 84]
				Methacrolein (Methacrylaldehyde)	78-85-3	[66, 80]
				Pentanal	110-62-3	[84]
		Alkane		2- methylbutanal	96-17-3	[81]
				2,3,3-trimethylpentane	560-21-4	[80]
				2,3,5-trimethylhexane	1069-53-0	[81]
				2,4-dimethyl heptane	2213-23-2	[80]
				2,4-dimethyl-1-heptane	19549-87-2	[80]
				2-methyl-2-butenal	1115-11-3	[66, 80]
				Octane	111-65-9	[66]
		Aromatic		Styrene	100-42-5	[85]
				Toluene	108-88-3	[85]
		Ester		Butyl acetate	123-86-4	[66, 81, 86]
		Ketone		2-butanone	78-93-3	[80, 81]
			2-pentanone	107-87-9	[66]	
	Acetone		67-64-1	[66, 82]		

Disease	Sample source	Chemical family	VOC	CAS number	Ref
		Nitrile	Acetonitrile	75-05-8	[80]
	Saliva	Alcohol	2-ethyl-1-hexanol	104-76-7	[87]
Melanoma	Skin	Alcohol	1-Eicosanol	629-96-9	[88]
			1-Hexadecanol	36653-82-4	[88, 89]
		Aldehyde	Decanal	112-31-2	[88]
			Nonanal	124-19-6	[88, 89]
		Alkane	1-iodo nonane	4282-42-2	[88]
			2,4-dimethyl heptane	2213-23-2	[88]
			4,7dimethyl-undecane	17301-32-5	[88]
			Cyclohexane, ethyl	1678-91-7	[88]
			Decane	124-18-5	[88, 89]
			Decane, 4-methyl	2847-72-5	[88, 89]
			Dodecane	112-40-3	[88, 89]
			Pentane, 2,3,4-trimethyl	565-75-3	[88]
			Undecane	1120-21-4	[88, 89]
		Alkene	1-hexadecene	629-73-2	[88]
		Amide	Formamide	75-12-7	[88]
			Adenosine, 5'-amino-5'-deoxy	14365-44-7	[88]
		Aromatic	1,3,5-trimethyl-benzene (Mesitylene)	108-67-8	[88, 89]
			Bis(2-ethylhexyl) phthalate	117-81-7	[88, 89]
		Ester	1,2-Benzenedicarboxylic acid, diisooctyl ester	117-84-0	[88]
		Ester	Isopropyl Palmitate	142-91-6	[88, 89]
Phthalic acid, isobutyl 4-octyl ester	314-84-7		[88]		

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			2-butoxy-ethanol	111-76-2	[88]
			Ethylene oxide	75-21-8	[88, 89]
		Nitrile	2-Isopropylamino-4-methylbenzotrile	28195-00-8	[88]
		Organosulphur	N-Morpholinomethyl-isopropyl-sulfide	77422-34-5	[88]
		Other	1,3-Cyclopentadiene, 5-(1-methylethylidene)-	2175-91-9	[88]
			2-Ethoxyethyl acrylate	106-74-1	[88]
			2-Ethylhexyl trans-4-methoxycinnamate	83834-59-7	[88]
			Benzaldehyde, 4-methoxy	123-11-5	[88]
			Dichlorodifluoromethane	75-43-4	[88]
				Spiro[bicyclo[2.2.1]hept-5-ene-2,1'-cyclopropane]	6572-50-5
Multiple sclerosis	Breath	Aldehyde	Decanal	112-31-2	[90]
			Hexanal	66-25-1	[91]
			Nonanal	124-19-6	[90]
		Alkane	5-methyl-undecane	1632-70-8	[91]
		Alkene	Heptadecane	629-78-7	[90]
		Ketone	Acetophenone	98-86-2	[90]
		Organosulphur	Sulfur dioxide	7446-09-5	[90]
Parkinson	Breath	Aromatic	1-methyl-3-(1-methylethyl)-benzene (m-Cymene)	535-77-3	[2]
	Breath (human and rats)	Alkane	Hexadecane	544-76-3	[2] [92]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			2,3,5-trimethylhexane	1069-53-0	[2, 92]
			2,3,6,7-tetramethyl-octane	52670-34-5	[2, 92]
			2,3-dimethyl-heptane	3074-71-3	[2, 92]
			3,7-dimethyl-decane	17312-54-8	[2, 92]
			5-ethyl-2-methyl-octane	62016-18-6	[2, 92]
		Aromatic	1-methyl-3-(1-methylethyl)-benzene (m-Cymene)	535-77-3	[2, 92]
			Butylated hydroxytoluene	128-37-0	[2, 92]
			Ethylbenzene	100-41-4	[2, 92]
			Styrene	100-42-5	[2, 92]
		Other	Decamethyl-cyclopentasiloxane	541-02-6	[2, 92]
		Prostate Cancer	Breath	Alkane	2,2-dimethyl-decane
Aromatic	P-xylene			106-42-3	[12]
	Toluene			108-88-3	[12]
Nitrile	2-amino-5-isopropyl-8-methyl-1-azulenecarbonitrile			93946-48-6	[12]
Pulmonary Arterial	Breath	Alcohol	Ethanol	64-17-5	[93]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
Hypertension			Isopropyl alcohol	67-63-0	[93]
		Aldehyde	Acetaldehyde	75-07-0	[93]
			Benzaldehyde	100-52-7	[94]
		Alkane	Pentane	109-66-0	[93]
		Alkene	1-decene	872-05-9	[93]
			1-octene	111-66-0	[93]
			2-nonene	2216-38-8	[93]
		Amine	Ammonia	7664-41-7	[93]
		Aromatic	1-methyl-4-(1-methylethyl)-benzene (p-Cymene)	99-87-6	[94]
			Aniline	62-53-3	[94]
			Benzenamine, N-ethyl-	103-69-5	[94]
			Benzothiazole	95-16-9	[94]
		Ester	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	N/A	[94]
			Propanoic acid, 2-methyl-, 3-hydroxyhexyl ester	N/A	[94]
			Tetrahydro-2, 2, 4, 4-tetramethyl furan	3358-28-9	[94]

Disease	Sample source	Chemical family	VOC	CAS number	Ref
		Ketone	2,2-dihydroxy-1-phenyl-ethanone	1075-06-5	[94]
			4-Methyl-2-pentanone	1108-10-1	[94]
			P-menthone	89-80-5	[94]
		Other	1, 6-dioxacyclododecane-7, 12-dione	777-95-7	[94]
			1-methyl-3-(1-methylethyl)-benzene (m-Cymene)	535-77-3	[94]
			2-menthene	2230-85-5	[94]
Renal disease	Breath	Alcohol	Isopropyl alcohol	67-63-0	[95]
		Alkane	2,4-dimethyl heptane	2213-23-2	[95]
			Isononane	34464-40-9	[95]
			Nonane	111-84-2	[95]
		Aromatic	Ethylbenzene	100-41-4	[95]
			Styrene	100-42-5	[95]
Other	Methylene chloride	75-09-2	[95]		
Rheumatoid arthritis	Breath	Alkane	Pentane	109-66-0	[96]
Schizophrenia	Breath	Alkane	Ethane	74-84-0	[97]
			Pentane	109-66-0	[97]
		Organosulphur	Carbon disulfide	75-15-0	[97]
Tuberculosis	Breath	Alcohol	2-butyl-1-octanol	3913-02-8	[98]
		Alkane	Dodecane, 4-methyl	6117-97-1	[98]

Disease	Sample source	Chemical family	VOC	CAS number	Ref		
			Tridecane	629-50-5	[98, 99]		
		Aromatic	1,3,5-trimethyl-benzene (Mesitylene)	108-67-8	[98, 99]		
			Methyl nicotinate	93-60-7	[100, 101]		
	In vitro	Alcohol		1-hexanol	111-27-3	[102, 103]	
				2-Phenylethanol	60-12-8	[103, 104]	
		Aldehyde		3-methylbutanal	590-86-3	[105]	
		Alkane		Heptane ,2,2,4,6,6-pentamethyl-	13475-82-6	[105]	
		Aromatic		4-methylanisol	104-93-8	[102, 104]	
				Ethyl benzoate	93-89-0	[102, 104]	
				Methyl 2-aminobenzoate	134-20-3	[102, 104]	
				Methyl benzoate	93-58-3	[102, 104]	
				Methyl nicotinate	93-60-7	[100, 102-104]	
				Methyl p-anisate	121-98-2	[100, 102-104]	
				Methyl salicylate	119-36-8	[102, 104]	
				O-Phenylanisole (2-Methoxybiphenyl)	86-26-0	[100, 102-104]	
		Ester		Methyl phenylacetate	101-41-7	[100, 102-104]	
		Other		4-Pentanolide	542-28-9	[102, 104]	
				Camphor	76-22-2	[102-104]	
		Urine	Alcohol		3-pentanol	584-02-1	[106]
			Aromatic		1-methyl-4-(1-methylethyl)-benzene (p-Cymene)	99-87-6	[106]
				2,6-dimethylstyrene	2039-90-9	[106]	

Disease	Sample source	Chemical family	VOC	CAS number	Ref
			O-xylene	95-47-6	[106]
		Ester	Isopropyl acetate	108-21-4	[106]

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