

Supporting Information for:

Sensors for Detecting Pulmonary Diseases from Exhaled Breath

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Table S1- classification of VOCs based on pulmonary disease.

| Disease | Chemical family | VOC | Reference | |
|-------------|-----------------------|---------------|---|------|
| Lung cancer | Alcohol | 4-penten-2-ol | [1] | |
| | | Ethanol | [2], [3, 4] | |
| | | Methanol | [5] | |
| | Aldehyde | Butanal | [6, 7] | |
| | | Formaldehyde | [8, 9] | |
| | | Heptanal | [6],[10, 11, 12] | |
| | | Hexanal | [4],[6],[10, 11, 12] | |
| | | Nonanal | [6],[9] | |
| | | Octanal | [3, 9, 13] | |
| | | Pentanal | [6],[9] | |
| | | propanal | [6, 7] | |
| | | Alkane | 1,1,2-trichloro-1,2,2-trifluoro- ethane | [14] |
| | | | 1-methyl-2-pentyl-cyclopropane | [11] |
| | 2,3,4-trimethylhexane | | [15] | |
| | 2,4-dimethyl heptane | | [11] | |
| | 2-methylheptane | | [11] | |
| | 2-methylhexane | | [16] | |
| | 2-methyl-pentane | | [17] | |
| | 3,3-dimethyl pentane | | [15] | |
| | 3-methyl-hexane | | [16] | |
| | 3-methyl-nonane | | [11] | |
| | 3-methyl-octane | | [11, 17] | |
| | 3-methyltridecane | | [16] | |
| | 4-methyl-octane | | [16] | |
| | 5-methyl-decane | | [16] | |
| | 7-methyl-tridecane | | [16] | |
| | Butane | | [2, 4, 18] | |
| | Cyclohexane | | [4] [11], [4, 19] | |
| | Decane | | [11, 17] | |
| | Decane, 4-methyl | | [20] | |
| | Dodecane | | [15] | |
| | Heptane | [10, 17, 18] | | |

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| | | Heptane ,2,2,4,6,6- pentamethyl- | [11] |
| | | Methyl-cyclopentane | [1, 11] |
| | | Methylcyclopropane | [21] |
| | | Octane | [3], [10] |
| | | Pentane | [10], [4, 17] |
| | | Trichlorofluoro-methane | [11] |
| | | Undecane | [10, 11], [8], [22] |
| | Alkene | 1,3-butadiene,2-methyl- isoprene | [11] |
| | | 1,5,9-trimethyl-1,5,9-cyclododecatriene | [20] |
| | | 1-heptene | [11], [17, 18] |
| | | 1-hexene | [21] |
| | | 2,3-hexadiene | [1] |
| | | 5,5-dimethyl-1,3-hexadiene | [1] |
| | | Isoprene | [2], [4, 10, 17] |
| | Aromatic | 1,1-(1,2-cyclobutanediyl)bis- ,cis- benzene | [1] |
| | | 1,1'-(1-butenylidene)bis benzene | [1] |
| | | 1,2,3,4-tetrahydro-9-propyl-anthracene | [1] |
| | | 1,2,4,5-3,3,6,6-tetraphenyl- tetroxane | [1] |
| | | 1,2,4-trimethyl benzene | [11, 17] |
| | | 1,4-dimethylbenzene (p-xylene) | [11] |
| | | 10,11-dihydro-5H-dibenzo- (B,F)-azepin | [20] |
| | | 1-methyl-4-(1-methylethyl)- benzene (p-Cymene) | [15] |
| | | 1-oxybis-benzene | [20] |
| | | 2,2-diethyl-1,1-biphenyl | [20] |
| | | 2,3-dihydro-1,1,3-trimethyl-3- phenyl-1-H-indene | [20, 23] |
| | | 2,5-dimethyl furan | [7, 20, 23] |
| | | 2-ethyl-9,10-anthracenediol | [1] |
| | | Aniline | [1] |
| | | Benzene | [2, 4, 10, 11, 17, 22] |
| | | Benzophenone | [1] |
| | | Diethylbenzene-1,2- dicarboxylate | [20] |
| | | Ethyl-4-ethoxybenzoate | [20, 23] |
| | | Ethylbenzene | [5] |
| | | O-toluidine | [1, 24] |
| | | Propyl benzene | [10, 11, 22] |
| | | Styrene | [4, 11, 17, 22] |
| | | Toluene | [15, 17] |
| | Ester | 2,2,4-trimethyl-pentan-1,3-dioldiisobutyrate | [20] |

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| | | Propanoic acid, 2,2,4-trimethyl- 3-carboxyisopropyl, isobutylester | [1] |
| | | 2-methoxy-2-methyl-propane | [1] |
| | Ketone | 2,4-dimethyl-3-pentanone | [20] |
| | | 2,5-dimethyl-2,4-hexanedione | [20] |
| | | 2-butanone | [25] |
| | | 2-methyl-3-hexanone | [1] |
| | | 3-hydroxy-2-butanone (Acetoin) | [25, 26, 27] |
| | | Acetone | [4, 10, 25, 28] |
| | | A-isomethyl ionone | [1] |
| | Nitrile | Acetonitrile | [7] |
| | Organosulphur | 1-(methylthio)-(E)-1-propene | [1] |
| | | 1,1-[1- (ethylthio)propylidene]bis-benzene | [1] |
| | | Carbon disulfide | [16] |
| | | Dimethyl sulphide | [20] |
| | Other | 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | [1] |
| | | 2,2,7,7-tetramethyltricyclo[6.2.1.0(1,6)]undec-4-en-3-one | [1] |
| | | 2,5-2,6-bis(1,1-dimethylethyl)-cyclohexadiene-1,4-dione | [20] |
| | | 2,6-bis(1,1-dimethylethyl)-4-ethylidene-2,5-cyclohexadien- 1-one | [1] |
| | | 2-methyl-,1-(1,1-dimethylethyl)-2-methyl-1,3- propanediyl ester | [20] |
| | | 5- (Ethoxycarbonyl)bicyclo[3.2.2]nonane-1-carboxylic acid | [1] |
| | | 5-isopropenyl-2-methyl-7-oxabicyclo[4.1.0]heptan-2-ol | [1] |
| | | 7,7-trimethyl-(1S)-bicyclo[2.2.1]heptan-2-one | [1] |
| | | Camphor | [1] |
| | | P-menth-1-en-8-ol (alpha- | [1] |
| Pulmonary Arterial Hypertension (PAH) | | Alcohol | Ethanol |
| | Isopropyl alcohol | | [29] |
| | Aldehyde | Acetaldehyde | [29] |
| | | Benzaldehyde | [30] |
| | Alkane | Pentane | [29] |
| | Alkene | 1-decene | [29] |
| | | 1-octene | [29] |
| | | 2-nonene | [29] |
| | Amine | Ammonia | [29] |
| | Aromatic | 1-methyl-4-(1-methylethyl)- benzene (p-Cymene) | [30] |
| | | Aniline | [30] |
| | | Benzenamine, N-ethyl- | [30] |
| | | Benzothiazole | [30] |

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| | Ester | Propanoic acid, 2-methyl-, 3- hydroxy-2,4,4-trimethylpentyl ester | [30] |
| | | Propanoic acid, 2-methyl-, 3-hydroxyhexyl ester | [30] |
| | | Tetrahydro-2, 2, 4, 4- tetramethyl furan | [30] |
| | Ketone | 2,2-dihydroxy-1-phenyl- ethanone | [30] |
| | | 4-Methyl-2-pentanone | [30] |
| | | P-menthone | [30] |
| | Other | 1, 6-dioxacyclododecane-7, 12- dione | [30] |
| | | 1-methyl-3-(1-methylethyl)- benzene (m-Cymene) | [30] |
| | | 2-menthene | [30] |
| Asthma | Alkane | Ethane | [31] |
| | | Pentane | [32] |
| | Amine | Ammonia | [33, 34] |
| | Nitrile | NO | [35, 36] |
| | Other | 8-isoprostane | [37] |
| Hydrogen peroxide | | [38] | |
| Chronic obstructive pulmonary disease (COPD) | Aldehyde | Heptanal | [39] |
| | | Hexanal | [39] |
| | | Malondialdehyde | [39] |
| | | Nonanal | [39, 40] |
| | Alkane | 2,4,6-Trimethyl-decane | [40] |
| | | 2,6-dimethyl-heptane | [40] |
| | | 4,7dimethyl-undecane | [40] |
| | | 4-methyl-octane | [40] |
| | | Ethane | [41] |
| | | Hexadecane | [40] |
| | | Octadecane | [40] |
| | Undecane | [40] | |
| | Alkene | Isoprene | [40] |
| | Nitrile | Benzonitrile | [40] |
| | Other | NO | [42] |
| 3,7-Dimethyl 1,3,6-octatriene | | [40] | |
| Hydrogen peroxide | | [43] | |
| Terpineol | | [40] | |
| Tuberculosis | Alcohol | 2-butyl-1-octanol | [44] |
| | Alkane | Dodecane, 4-methyl | [44] |
| | | 629-50-5 | [44, 45] |
| | | 108-67-8 | [44, 45] |
| Aromatic | 93-60-7 | [46, 47] | |
| | Nitrile | NO | [48, 49] |
| Cystic fibrosis | Organosulphur | Carbonyl sulfide | [50] |
| | Pneumoconiosis | Ketone | Acetone |
| Alkane | | Pentane | [51] |
| | | Hexane | [51] |
| | | Cyclohexane, 1-methylene-3-(1-methylethyl) | [51] |
| | | Bicyclo[4.1.0]heptane, 3,7,7-trimethyl- | [51] |
| Aldehyde | | Butanal, 3-methyl- | [51] |
| Alcohol | Phenylethyl alcohol | [51] | |
| Other | Methyl chloride | [51] | |

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| | | 1,4-Cyclohexadiene, 1-methyl-4-(1-methyl) | [51] |
| Obstructive Sleep Apnea Syndrome (OSAS) | Alkanes | Hexane | [52] |
| | | Heptane | [52] |
| | | Octane | [52] |
| | | Nonane | [52] |
| | | Decane | [52] |
| | Alkenes | Isoprene | [52] |
| | Ketones | Acetone | [52] |
| | Alcohols | Ethanol | [52] |
| | Aromatics | Benzene | [52] |
| | | Toluene | [52] |
| | | Ethylbenzene | [52] |
| | | p-Xylene | [52] |
| | | Phenylacetic acid | [52] |
| Alicyclic hydrocarbons | | [52] | |
| | | Cyclohexane | [52] |

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