Supporting Information for

"On-line analysis of exhaled breath"

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Table S1: Reported volatile organic compounds detected by on-line analysis of exhaled breath

Table S1: Reported volatile organic compounds detected by on-line breath analysis methods based on a literature search. The table is grouped into 17 compound classes (small volatiles (e.g. NO), alcohols, aldehydes, alkanes/alkenes/alkynes, amino acids, benzenoids, benzothiazoles, carboxylic acids, esters, fatty acids, furans, indoles, ketones, sulphur containing compounds, terpenes, inorganic compounds and "others"). The references for each compound are listed and annotated by detection method and identification confidence. **Literature search:** This table was created based on a literature search with web of science with the following criteria: TI=(breath OR exhaled OR exhalome) AND TS=(online OR on-line OR realtime OR real-time) AND TS=(subjects OR human OR healthy) OR Selected Ion Flow Tube Mass Spectrometry OR secondary electrospray ionization mass spectrometry OR ion mobility separation) AND DOCUMENT TYPES: (article) AND Timespan=all years. Search date: 06.03.2019; search result: 146 original articles. **Identification levels:** For mass spectrometry methods the identification levels 1-5 from chapter 4.4 from the manuscript were taken. Optical methods or sensor based methods were categorized as either measured with or without reference standards. **Abbreviations:** Mass spectrometry methods: Proton-transfer-reaction mass spectrometry (PTR-MS), Selected-ion flow-tube mass spectrometry (SIFT-MS), Secondary electrospray ionization-mass spectrometry (SESI-MS), High-resolution mass spectrometry (HRMS), Time-of-flight mass spectrometry (TOF-MS), confined direct analysis in real time time-of-flight mass spectrometry (cDART-TOF-MS), Active Capillary Plasma Ionisation (ACPI), Resonance-enhanced multiphoton ionization-mass spectrometry (REMPI-MS), acetone-assisted negative photoionization ion mobility spectrometer (AANP-IMS); Optical methods: Cavity ringdown spectroscopy (CRDS), Cavity-enhanced Absorption Spectroscopy (CE-AS), Cavity-enhanced optical frequency comb spectroscopy (CE-OFCS), Photoacoustic Spectroscopy (PAS), Tunable diode laser absorption spectroscopy (TDLAS), Infrared-luminescence spectroscopy (ILS), Infrared Laser-Spectroscopic (IR-LS), Mid-Infrared Laser Spectroscopy (MI-LS), Near-Infrared Laser Spectroscopy (NIR-LS), Near-Infrared Cavity Ring-Down Spectroscopy (NIR-CRDS), Laser Magnetic Resonance Spectroscopy (LM-RS), Laser-Induced Fluorescence Spectroscopy (LI-FS), Laser Based Absorption Spectroscopy (OPO OA-LCOS), Infrared Cavity Leak-Out Spectroscopy (IR-CLOS), Quantum Cascade Laser Spectroscopy (QCL), Integrated Cavity Output Spectroscopy (OA-LCOS), Laser spectroscopy (LS); Sensors: Luminescence Sensor (LS sensor), Quantum Cascade Laser-Based Sensors (QCL sensors), Optical fiber sensor (OF sensor).

Compound class (Method class)	Compound	Method (Identification level)
Small volatiles (mass spectrometry, optical methods, chemical sensors)	Acetonitrile	PTR-MS (ID2[1], ID4[2 3], ID5[4]), PTR-TOF-MS (ID4[5 6])
	Ammonia	SIFT-MS (ID2[7 8 9], ID5[10 11 12 13 14 15]), PTR-TOF-MS (ID4[5 6 16]), PTR-MS (ID4[1], ID5[17 18]), cDART-TOF-MS (ID4[19]), CRDS (with[20]/without standard[21 22]), CE-AS, CE-OFCS (without standard[23]), PAS (ID1[24])
	Carbon monoxide (CO)	PTR-TOF-MS (ID4[5]), CRDS (without standard[21]), CE-OFCS without standard[25]), QCL (with standard[26]), QCL sensors (with standards[27]), TDLAS (without standard[28])
	Carbon monoxide (^{12}CO, ^{13}CO)	MI-LS (with standards[29])
	Carbon dioxide (CO_2)	PTR-TOF-MS (ID4[5]), PTR-MS (ID4[2]), TDLAS (without standard[30]), CRDS (without standard[21]) ILS (without standard[31]), OPO OA-LCOS (without standard[32]),
	Carbondioxide ($^{12}CO_2$, $^{13}CO_2$)	TDLAS (with standard[33]), CE-OFCS (with standard[25]), QCL (without standard[34])

Small volatiles (continued)	Hydrogen Cyanide	SIFT-MS (ID2[7 35], ID5[12]), CRDS (with standard[20])
	Hydrogen Sulphide	PTR-TOF-MS (ID4[6])
	Nitrogen	CRDS (with standard[21]),
	Nitrogen Oxide	REMPI-MS (ID3[36]), TDLS (without standard[30]), CRDS (without standard[21]), CE-AS (with standard[23 37]), LM-RS (with standard[38]), QCL (with standard[39 40], without standard[41]), PAS (without standard[23 42 43]),
	Nitrogen Oxide (^{14}NO, ^{15}NO)	LI-FS (with standard[44]), IR-LS (with standard[45])
	Oxygen	LS sensor (without standard[31]), CRDS (without standard[21])
	Water (H_2O)	SIFT-MS (ID2[8], ID5[12 46]), CRDS (without standard[21]), CE-OFCS (with standard[25]), OPO OA-LCOS (without standard[32])
Alcohols (mass spectrometry)	1,2-Propanediol; 1,3-Butanediol	PTR-MS (ID5[18])
	2-Propyl-1-Pentanol	PTR-TOF-MS (ID4[5])
	Butanol	PTR-TOF-MS (ID4[5 47]), PTR-MS (ID5[18])
	Ethanol	SIFT-MS (ID2[7 8 9], ID5[12 13 48 49 50]), PTR-MS (ID2[1 51], ID5[52 53]), PTR-TOF-MS (ID4[5 16 47]), CRDS (without standard[21]), OA-LCOS (without standard[54])
	Heptadienol	PTR-TOF-MS (ID4[55])
	Isopropanol	PTR-TOF-MS (ID4[6])
	Methanol	PTR-MS (ID2[1], ID5[18]), PTR-TOF-MS (ID4[5 55 56 47]), SIFT-MS (ID2[7 9], ID5[12 57]), CRDS (without standard[21])
	Phenol	cDART-TOF-MS (ID1[19]), PTR-TOF-MS (ID4[47])
	Phenyl Ethanol	PTR-MS (ID5[58])
	Propanol	SIFT-MS (ID2[59 7 9 12], ID5), PTR-MS (ID5[18]), CRDS (without standard[21])
Aldehydes (mass spectrometry)	3-Methyl Benzaldehyde	cDART-TOF-MS (ID1[19])
	Acetaldehyde	PTR-MS (ID2[51], ID5[18 60 49], PTR-TOF-MS (ID4[5 47]), SIFT-MS (ID2[8 9], ID5[12 48 49 50]), cDART-TOF-MS (ID4[19]), TDLAS (with standard[61])
	Acrolein	PTR-MS (ID2[51], ID5[18])
	Butanal	PTR-MS (D2[51], ID4[3])
	Decanal; E-2-Butenal	PTR-MS (ID2[51])

Aldehydes (continued)	Formaldehyde	PTR-MS (ID2[51]), SIFT-MS (ID2[7 9], ID5 [12])
	Glycoaldehyde	PTR-MS (ID5[18])
	Heptanal	PTR-MS (ID2[51]), PTR-TOF-MS (ID4[16]),
	Hexanal	PTR-MS (ID2[51], ID5[60])
	Methacrolein, Methylglyoxal	PTR-MS (ID5[18])
	Methylpentenal	ACPI-MS (ID5[62])
	Methylpropenal	PTR-TOF-MS (ID4[47])
	Nonanal	cDART-TOF-MS (ID4[19]), PTR-MS (ID2[51]), PTR-TOF-MS(ID5[5])
	Octanal	PTR-MS (ID2[51])
	Pentanal	PTR-MS (ID2[51]), PTR-TOF-MS (ID4[16])
	Propanal	PTR-MS (ID2[51])
	Pyrrolidine Carboxaldehyde	ACPI-MS (ID5[62])
Alkanes/Alkenes/Alkynes (mass spectrometry, optical methods, chemical sensors)	2-Methyl-1-Butene	PTR-TOF-MS (ID4[47])
	2,4-Dimethyl-1-Heptene	cDART-TOF-MS (with standard[19])
	Acetylene	CRDS (with standard[20]), NIR-CRDS (without standard[63]), NIR-LS (without standard[64]),
	Ethane	TDLAS (with standard[65]), CE-AS (with standard[37]), IR-CLOS (with standard[66]), LS (with standard[67]), OF sensor (with standard[68]), CRDS (without standard[21]), OPO OA-LCOS (without standard[32]),
	Pentane, Heptane, Octane, Decane	OF sensor (with standard[68])
	Ethylene	Chemical sensor (with standard[69]), PAS (with standard[65])
	Methane	SIFT-MS (ID5[46]), CRDS (without standard[21]), CE-OFCS (with standard[25]), OPO OA-LCOS (without standard[32])
	Nonene; Octene	ACPI-MS (ID5[62])
	Pentane	SIFT-MS (ID5[46]), CRDS (without standard[21])
	Trans-2-Butene	PTR-TOF-MS (ID4[47])
Amino acids (mass spectrometry)	Alanine; Glycine; Leucine;	SESI-HRMS (ID1[70]); SESI-MS(ID3[70])

Amino acids (continued)	Lysine; Ornithine; Phenylalanine; Proline; Valine	
Benzenoids (mass spectrometry, optical methods)	1,2-Dichlorobenzene; 1,2,4,-Trichlorobenzene	PTR-MS (ID2[51])
	Aniline	cDART-TOF-MS (ID4[19])
	Anthranilate	SESI-MS (ID4[71])
	Benzaldehyde	cDART-TOF-MS (ID1[19])
	Benzene	PTR-MS (ID2[51], ID5[18]), PTR-TOF-MS (ID4[47]), Optical fiber sensor (ID1[68])
	Benzol	PTR-MS (ID4[2])
	Ethyl-4-Ethoxybenzoate	cDART-TOF-MS (ID1[19])
	Methyl Propyl Sulphide	PTR-TOF-MS (ID4[6])
	O-Xylene	PTR-MS (ID2[51])
	Propofol	PTR-MS (ID1[72]), SIFT-MS (ID3[73]), IMR-MS(ID4[74]), AANP-IMS (with standard[75])
	Propyl-4-Methylbenzoate	cDART-TOF-MS (ID1[19])
	Styrene	Optical fiber sensor (ID1[68])
	Toluene	PTR-MS (ID2[51]), PTR-TOF-MS (ID4[5]), SIFT-MS (ID5[11]), Optical fiber sensor (ID1[68])
	Xylene	SIFT-MS (ID5[11])
Benzothiazoles (mass spectrometry)	2-(4-Morpholinyl)-Benzothiazole	SESI-MS (ID1[76])
	2-Aminobenzothiazole; 2-Hydroxybenzothiazole; 2-Mercaptobenzothiazole; 2-Methylthiobenzothiazole	SESI-MS (ID1[76])
	Benzothiazole	SESI-MS (ID1[76], ID4[77]), cDART-TOF-MS (ID4[19])
Carboxylic acids (mass spectrometry)	3-Hydroxypentanoic Acid; 3-Methyl-2-Oxobutanoic Acid; 3-Methylbutanoic Acid; 4-Methyl-2-Oxopentanoic Acid	ACPI-MS (ID4[62])

Carboxylic acids (continued)	5-Hydroxy-L-Tryptophan	SESI-MS (ID4[71])
	Acetic Acid	PTR-MS (ID2[1 18]), SIFT-MS (ID2[59]) PTR-TOF-MS (ID4[5]),
	Aconitic Acid	SESI-MS
	Decanedioic Acid; Dodecanedioic Acid	SESI-MS (ID1[78])
	Erythronic Acid	SESI-MS (ID4[79])
	Formic Acid	PTR-TOF-MS (ID4[5 6 47])
	Fumaric Acid	SESI-MS (ID1[80])
	Glyceric Acid	SESI-MS (ID4[79])
	Heptanedioic Acid	SESI-MS (ID1[78])
	Hexanedioic Acid	SESI-MS (ID3[78])
	Lactate	SESI-MS (ID4[79])
	Malic Acid	SESI-MS (ID1[80])
	N-Methyl-Alpha-Aminoisobutyric Acid	ACPI-MS (ID4[62])
	Nonanedioic Acid; Pentadecanedioic Acid; Tridecanedioic Acid	SESI-MS (ID3[78])
	Octanedioic Acid; Pentanedioic Acid; Undecanedioic Acid; Tetradecanedioic Acid	SESI-MS (ID1[78])
	Propionic Acid	PTR-TOF-MS (ID4[6 47]); PTR-MS (ID5[18])
	Succinic Acid	SESI-MS (ID1[80])
Esters (mass spectrometry)	4-Methyl-2-Hydroxy-2-Phenylpropyl Ester	cDART-TOF-MS (ID1[19])
	Benzyl Acetate; Benzyl Propionate	cDART-TOF-MS (ID1[19])
	Ethyl Acetate; Ethyl Butanoate	PTR-MS (ID5[58])
	Isobutyl Acetate; Isopentyl Acetate	cDART-TOF-MS (ID4[19])
	Methyl Acetate	PTR-MS (ID5[18])

Fatty acids (mass spectrometry)	10-Hydroxydecanoic Acid; 10-Oxodecanoic Acid; 11-Hydroxyundecanoic Acid; 11-Oxoundecanoic Acid; 8-Hydroxyoctanoic Acid	SESI-MS (ID1[78])
	12-Amino-Dodecanoic Acid	SESI-MS (ID4[79])
	13-Hydroxytridecanoic Acid; 13-Oxotridecanoic Acid; 14-Hydroxytetradecanoic Acid; 14-Oxotetradecanoic Acid; 15-Hydroxypentadecanoic Acid; 15-Oxopentadecanoic Acid; 5-Hydroxypentanoic Acid; 5-Oxopentanoic Acid; 6-Hydroxyhexanoic Acid; 7-Hydroxyheptanoic Acid	SESI-MS (ID4[78])
	12-Oxododecanoic Acid	SESI-MS (ID1[78])
	6-Oxohexanoic Acid; 7-Oxoheptanoic Acid; 8-Oxooctanoic Acid; 9-Hydroxynonanoic Acid; 9-Oxononanoic Acid	SESI-MS (ID3[78])
	Butyric Acid	PTR-TOF-MS (ID4[47]), SESI-MS (ID2[81])
	Docosahexanoic Acid; Hydroxyoctanoic Acid	SESI-MS (ID4[77])
	Fatty Acids (C4:1 - C19:0)	ACPI-MS (ID5[62])
	Hexanoic Acid	SESI-MS (ID2[81])
	Isobutyric Acid; Isovaleric Acid	SESI-MS (ID2[81])
	Nonanoic Acid; Oxohexanoic Acid	PTR-TOF-MS (ID4[5]); SESI-MS (ID4[77])

Fatty acids (continued)	Propanoic Acid; Valeric Acid	SESI-MS (ID2[81])
Furans (mass spectrometry)	Dihydro-4-Methyl-2(3H)-Furanone	PTR-TOF-MS (ID4[5])
	Furan	PTR-MS (ID4[2,3]), PTR-TOF-MS (ID4[6,47]), cDART-TOF-MS (ID4[19])
Indoles (mass spectrometry)	3-Methyldioxyindole; 5-Hydroxyindoleacetaldehyde; 6-Hydroxymelatonin	SESI-MS (ID4[71])
	5-Methoxyindoleacetate	SESI-MS (ID2[71])
	Indole	SESI-MS (ID4[82])
	Indole-3-Acetate	SESI-MS (ID1[71])
	N-Acetylserotonin	SESI-MS (ID4[71])
Ketones (mass spectrometry)	2-Butanone	PTR-MS (ID2[51]), PTR-TOF-MS (ID4[55])
	2,3-Butanedinone	cDART-TOF-MS (ID4[19])
	3-Hydroxykynurenine	SESI-MS (ID1[71])
	4-(2-Amino-3-Hydroxyphenyl)-2,4-Dioxobutanoate; 4-(2-Aminophenyl)-2,4-Dioxobutanoate	SESI-MS (ID4[71]), cDART-TOF-MS (ID4[19])
	Acetone	PTR-MS (ID2[1,51] , ID4[83,2,3], ID5[84,4,18,17,60,58,85,86,53]), PTR-TOF-MS (ID4[5,6,47]), SESI-MS (ID2[7,8,9,87] , ID3[73], ID4[12,13,46,48,88,89,90,91]), SIFT-MS (ID5[50]), CRDS(with standard[92], without standard[21,93]), OA-LCOS (without standard[54]), OPO OA-LCOS (without standard[32]), cDART-TOF-MS (ID4[19]), Chemical sensor (ID1[94]), Chemical sensor (ID2[95])
	Alpha-Ketoglutaric Acid; Oxaloacetic Acid	SESI-MS (ID2[80])
	Hydroxyacetone	PTR-MS (ID5[18])
	Methyl Vinyl Ketone	PTR-TOF-MS (ID4[47])
	Pentanone	PTR-TOF-MS (ID4[55])
Sulphur containing (mass spectroemtry)	1(2)-Butanethiol; 2-Mercapto-Pyruvate; 2-Methyl-1(2)-Propanethiol; 3-Methyl-Thiopropionate	PTR-MS (ID5[18])

Sulphur containing (continued)	Allylmethylsulfide	PTR-TOF-MS (ID4[6 47])
	Capnine (2-Amino-3-Hydroxy-15-Methylhexadecane-1-Sulfonic Acid)	SESI-MS (ID2[79])
	Carbondisulfide	cDART-TOF-MS (ID4[19]), CE-AS (with standard[37])
	Dimethylsulfide	PTR-MS (ID2[1], ID5[18]), PTR-TOF-MS (ID5[5 6 47])
	Ethanethiol	PTR-MS (ID5[18])
	H2S	PTR-MS (ID4[2])
	Methanethiol	PTR-TOF-MS (ID4[5]), PTR-MS (ID5[18])
	Methylmercaptane	PTR-MS (ID4[96])
	Methylthio-Acetonitrile	cDART-TOF-MS (ID1[19])
	Propanethiol	PTR-MS (ID5[18])
	Thiourea	cDART-TOF-MS (ID4[19])
Terpenes (mass spectrometry)	1,8-Cineole	cDART-TOF-MS (ID4[19])
	Eucalyptol	PTR-MS (ID5[86])
	Isoprene	PTR-MS (ID2[1 51], ID4[2 3], ID5[4 17 58 60 85 84 97]), PTR-TOF-MS (ID4[5 6 16 47]), SIFT-MS (ID2[7 9 87], ID3[73], ID5[12 13 15]), cDART-TOF-MS (ID4[19]), IMR-MS (ID4[74 98]), CRDS (no standard[21])
	Limonene	PTR-TOF-MS (ID4[6]), cDART-TOF-MS (ID4[19])
	Menthol	cDART-TOF-MS (ID1[19])
Inorganic compounds (mass spectrometry)	Dichloramine; Monobromamine; Monochloramine	SIFT-MS (ID5[99])
	Nitrate/Nitric Acid; Phosphate/Phosphoric Acid; Silicate/Silicic Acid; Sulfate/Sulfuric Acid	SESI-MS (ID4[88])
Others (mass spectrometry, optical methods)	3 Hexylpyridine; 5-Hydroxykynurenine; n-Hydroxykynurenamine; n,n-Dihydroxyquinoline	SESI-MS (ID4[71 79])

Others (continued)	Dioctylphtalate	SESI-MS (ID2[90])
	Ethyl-2-Methylnicotinate	cDART-TOF-MS (ID1[19])
	Evocarpine	SESI-MS (ID2[79])
	Formyl-N-Acetyl-5-Methoxykynurenamine; L-Kynurenine; N-Formylkynurenine	SESI-MS (ID4[71])
	Nicotine	SESI-MS (ID2[79])
	Octylamine	SESI-MS (ID3[79])
	Polysiloxane	SESI-MS (ID4[88])
	Pyridine	SESI-MS (ID4[79 77])
	Ribose; Thioperamide	SESI-MS (ID4[79])
	Sevoflurane	AANP-IMS-VUV (ID1[75])
	Trimethylamine N-Oxide	PTR-MS (ID4[100])
	Tryptamine	SESI-MS (ID4[71])

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