NTD-GC-MS for characterization of lung diseases based on breath VOC profiles – Supplementary Material

Table S1 - Data regarding calibration method of gas mixtures (LOD = limit of detection, LOQ = limit of quantitation, ppbv = part per billion per volume, R^2 = determination coefficient, RSD = relative standard deviation).

Analyte	**LOD**	**LOQ**	**Linearity range**	**R^2**	**RSD (%)**
	(ppbv)				
2-Methylbutane	0.010	0.03	0.03-17.21	0.997	7.81
Pentane	0.105	0.315	0.315-17.49	0.990	7.60
Ethanol	0.430	1.29	1.29-3452.0	0.996	6.27
Isoprene	0.250	0.75	0.75-1886.0	0.993	10.00
2-Propanol	1.630	4.89	4.89-2616.0	0.992	9.61
2-Methylpentane	0.190	0.57	0.57-15.27	0.991	7.74
3-Methylpentane	0.001	0.003	0.003-15.43	0.996	6.95
1-Propanol	1.680	5.04	5.04-26.95	0.998	0.98
Methylcyclopentane	0.220	0.66	0.66-17.91	0.999	7.75
2-Butanone	0.001	0.003	0.003-22.5	0.996	7.29
Benzene	0.140	0.42	0.42-22.60	0.993	10.00
Acetoin	0.280	0.84	0.84-144.68	0.998	9.01
Toluene	0.001	0.003	0.003-19.03	0.991	6.17
Ethylbenzene	0.105	0.315	0.315-16.44	0.991	8.36
p-Xylene	0.100	0.30	0.30-16.32	0.991	7.45
Styrene	0.110	0.33	0.33-17.59	0.992	1.93
Decane	0.125	0.375	0.375-10.34	0.992	9.63
6-Methyl-2-heptanone	0.160	0.48	0.48-12.75	0.993	4.24
Isododecane	0.001	0.003	0.003-8.87	0.990	9.34
1,2,4-Trimethylbenzene	0.001	0.003	0.003-14.75	0.990	1.80
(E)-Ocimene	0.001	0.003	0.003-11.83	0.991	6.15
Limonene	0.001	0.003	0.003-12.44	0.990	6.45
m-Cymene	0.001	0.003	0.003-12.93	0.999	1.21
Benzonitrile	0.001	0.003	0.003-19.56	0.990	4.95
Phenol	1.430	4.29	4.29-11.46	0.993	9.48
Undecane	0.120	0.36	0.36-9.52	0.999	6.44
Dodecane	1.380	4.14	4.14-110.93	0.995	9.65
Terpineol	1.020	3.06	3.06-18.31	0.995	7.97
Tridecane	2.070	6.21	6.21-103.31	0.994	9.30

Table S2 - References which reported the targets selected in the present study as potential biomarker of lung diseases in breath samples, where: LC – lung cancer; COPD – chronic obstructive pulmonary disease [52,53,62–71,54,72–75,55–61].

Compound	Studied disease	Reference no. in Supplementary Material
2-Methylbutane	LC	[1]
Pentane	LC and COPD/COPD/LC	[2–4]
Ethanol	LC	[5]
Isoprene	LC/COPD/LC/LC and COPD/LC	[1,2,5,6]
2-Propanol	LC	[7]
2-Methylpentane	COPD/ Asthma/ LC and COPD/LC/LC	[2,4,8–10]
3-Methylpentane	LC	[4]
1-Propanol	LC	[1,4,11,12]
Methylcyclopentane	LC	[10]
2-Butanone	LC/COPD/LC	[1,4,8]
Benzene	COPD/Asthma/COPD/COPD/LC/ LC and COPD/LC	[2,8,10,11,13–15]
Acetoin	LC/LC	[1,16]
Toluene	COPD/COPD/LC and COPD/Asthma	[2,6,8,17]
Ethylbenzene	LC/LC and COPD/LC	[2,5,7]
p-Xylene	LC and COPD/LC/COPD	[2,13,18]
Styrene	LC and COPD/LC/LC	[2,10,19]
Decane	LC and COPD/LC/COPD	[2,10,20]
6-Methyl-2-heptanone	Wheeze	[21]
Isododecane	LC and COPD/LC	[2,10]
1,2,4-Trimethylbenzene	LC	[10]
E-Ocimene	COPD	[22]
Limonene	COPD	[20]
m-Cymene	Asthma	[23]
Benzonitrile	COPD	[22]
Phenol	COPD	[6,13]

Undecane	LC/COPD/LC	[1,19,22]
Dodecane	LC	[24]
Terpineol	COPD	[22]
Tridecane	COPD	[13]

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