

Compound and chemical classification	Author	Disease	Participants (N=)	Concentration change	Analytical technology
Aldehydes					
2-oxoglutaric acid semi-aldehyde	Bregy <i>et al</i> ⁶⁰	COPD	36	↑	SESI-MS
aspartic acid semi-aldehyde	Bregy <i>et al</i> ⁶⁰	COPD	36	↑	SESI-MS
Nonanal	Basanta <i>et al</i> ⁶⁷	COPD	71	↑	GC-TOF-MS
Nonanal	Callol-Sanchez <i>et al</i> ⁹⁰	Lung cancer	210	↑	GC-Tof-MS
Nonanal	Schleich <i>et al</i> ⁶³	Asthma	521	↑	GC-MS
Nonanal	Schleich <i>et al</i> ⁶³	Asthma	521	↑	GC-MS
Nonanal	Fowler <i>et al</i> ⁷³	Ventilator associated pneumonia	46	↑	TD/GC-Tof-MS
Pentadecanal	Basanta <i>et al</i> ⁶⁷	COPD	71	↑	GC-TOF-MS
Pentadecanal	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↓	GC-MS
Tetradecanal	Schnabel <i>et al</i> ¹⁰⁷	Ventilator associated pneumonia	100	↑	GC-Tof-MS
Undecanal	Basanta <i>et al</i> ⁶⁷	COPD	71	↑	GC-TOF-MS
Acrolein	Schnabel <i>et al</i> ¹⁰⁷	Ventilator associated pneumonia	100	↓	GC-Tof-MS
Esters					
Ethyl 2,2-dimethylacetoacetate	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↑	GC-MS
Linalylacetate	Gaida <i>et al</i> ⁶²	COPD	190	↑	TD-GC-MS

Ketones					
2-butanone	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↑	GC-MS
2-hexanone	Schleich <i>et al</i> ⁶³	Asthma	521	↓	GC-MS
2-pentanone	Allers <i>et al</i> ¹⁰⁸	COPD	58	↑	GC-APCI-MS
2-pentanone	Pizzini <i>et al</i> ⁶¹	COPD	54	↑	TD-GC-ToF-MS
4-heptanone	Pizzini <i>et al</i> ⁶¹	COPD	54	↑	TD-GC-ToF-MS
6-methyl-5-hepten-2-one	Pizzini <i>et al</i> ⁶¹	COPD	54	↓	TD-GC-ToF-MS
Acetone	Martinez <i>et al</i> ¹⁰⁹	COPD	61	↑	GC-IMS
Cyclohexanone	Pizzini <i>et al</i> ⁶¹	COPD	54	↑	TD-GC-ToF-MS
Cyclohexanone (CAS 108-94-1)	Westhoff <i>et al</i> ¹¹⁰	COPD		↑	GC-IMS
2-methyl cyclopentanone	Fowler <i>et al</i> ⁷³	Ventilator associated pneumonia	46	↑	TD-GC-ToF-MS
Organic acids					
11-hydroxyundecanoic acid	Bregy <i>et al</i> ⁶⁰	COPD	36	↓	SESI-MS
Acetic acid	Phillips <i>et al</i> ²⁰	COPD	182	↑	GC-MS
Butanoic acid	Basanta <i>et al</i> ⁶⁷	COPD	71	↓	GC-TOF-MS
Dodecanedioic acid	Bregy <i>et al</i> ⁶⁰	COPD	36	↓	SESI-MS
Oxoheptadecanoic acid	Bregy <i>et al</i> ⁶⁰	COPD	36	↓	SESI-MS
Pentanoic acid	Basanta <i>et al</i> ⁶⁷	COPD	71	↓	GC-TOF-MS

Alkanes					
3,7-dimethylnonane	Schleich <i>et al</i> ⁶³	Asthma	521	↓	GC-MS
Hexane	Schleich <i>et al</i> ⁶³	Asthma	521	↓	GC-MS
Undecane	Schleich <i>et al</i> ⁶³	Asthma	521	↑	GC-MS
2,6-Dimethyl-heptane	Van Berkel <i>et al</i> ¹¹¹	COPD	79	↑	GC-Tof-MS
4,7-Dimethyl-undecane	Van Berkel <i>et al</i> ¹¹¹	COPD	79	↑	GC-Tof-MS
4-Methyl-octane	Van Berkel <i>et al</i> ¹¹¹	COPD	79	↑	GC-Tof-MS
Hexadecane	Van Berkel <i>et al</i> ¹¹¹	COPD	79	↑	GC-Tof-MS
6-ethyl-2-methyl-Decane	Cazzola <i>et al</i> ¹¹²	COPD	34	↑	SPME- GC-MS
Decane	Cazzola <i>et al</i> ¹¹²	COPD	34	↑	SPME- GC-MS
Hexane, 3-ethyl-4-methyl-	Cazzola <i>et al</i> ¹¹²	COPD	34	↓	SPME- GC-MS
2 methyl-decane	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↑	GC-MS
2,6,10-trimethyl-dodecane	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↑	GC-MS
2,6,11-trimethyl-dodecane	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↑	GC-MS
5,5-Dibutylnonane	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↓	GC-MS
Dodecane	Schnabel ¹⁰⁷	Ventilator associated pneumonia	100	↓	GC-Tof-MS
Tetradecane	Schnabel ¹⁰⁷	Ventilator associated pneumonia	100	↑	GC-Tof-MS
Pentane	Olopade <i>et al</i> ⁵⁶	Asthma	40	↑	GC-MS

Ethane	Paredi <i>et al</i> ¹¹³	Asthma	40	↑	GC-MS
Butane	Phillips <i>et al</i> ²⁰	COPD	182	—	GC-MS
Butane	Schnabel <i>et al</i> ¹⁰⁷	Ventilator associated pneumonia	100	↑	GC-Tof-MS
2,4-dimethylheptane	Pizzini <i>et al</i> ⁶¹	COPD	54	↓	TD-GC-ToF-MS
2,6-dimethyloctane	Pizzini <i>et al</i> ⁶¹	COPD	54	↓	TD-GC-ToF-MS
2-methylhexane	Pizzini <i>et al</i> ⁶¹	COPD	54	↑	TD-GC-ToF-MS
cyclohexane	Pizzini <i>et al</i> ⁶¹	COPD	54	↑	TD-GC-ToF-MS
n-butane	Pizzini <i>et al</i> ⁶¹	COPD	54	↓	TD-GC-ToF-MS
n-Heptane	Pizzini <i>et al</i> ⁶¹	COPD	54	↑	TD-GC-ToF-MS
Heptane	Schnabel <i>et al</i> ¹⁰⁷	Ventilator associated pneumonia	100	↑	GC-Tof-MS
Heptane	Fowler <i>et al</i> ⁷³	Ventilator associated pneumonia	46	↓	GC-Tof-MS
Alkenes					
3- tetradecene	Schleich <i>et al</i> ⁶³	Asthma	521	↑	GC-MS
Pentadecene	Schleich <i>et al</i> ⁶³	Asthma	521	↑	GC-MS
Isoprene	Van Berkel <i>et al</i> ¹¹¹	COPD	79	↑	GC-Tof-MS
Isoprene	Phillips <i>et al</i> ²⁰	COPD	182	—	GC-MS
1-Pentene, 2,4,4-trimethyl-	Cazzola <i>et al</i> ¹¹²	COPD	34	↓	SPME – GC-MS
1,6-Dimethyl-1,3,5-heptatriene	Gaida <i>et al</i> ⁶²	COPD	190	—	GC-MS

3,5-heptatriene	Gaida <i>et al</i> ⁶²	COPD	190	—	GC-MS
4-ethyl-o-xylene	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↓	GC-MS
Nonadecane	Phillips <i>et al</i> ²⁰	COPD	182	—	GC-MS
Monoaromatics					
Benzene, 1,3,5-tri-tert-butyl-	Cazzola <i>et al</i> ¹¹²	COPD	34	↓	SPME – GC-MS
1-Ethyl-3-methyl benzene	Gaida <i>et al</i> ⁶²	COPD	190	↑	GC-MS
Benzene	Phillips <i>et al</i> ²⁰	COPD	182	—	GC-MS
Ethylbenzene	Schnabel <i>et al</i> ¹⁰⁷	Ventilator associated pneumonia	100	↑	GC-Tof-MS
Terpenes					
Limonene	Cazzola <i>et al</i> ¹¹²	COPD	34	↓	SPME – GC-MS
Terpinolene	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↑	GC-MS
Alcohols					
Cyclohexanol	Basanta <i>et al</i> ⁶⁷	COPD	71	↑	GC-TOF-MS
Bicyclo[2.2.2]octan-1-ol, 4-methyl - C9H16O	Brinkman <i>et al</i> ¹⁰⁴	Asthma	23	↑	GC-MS
Methanol CH3OH	Brinkman <i>et al</i> ¹⁰⁴	Asthma	23	↑	GC-MS
2-Propanol	Cazzola <i>et al</i> ¹¹²	COPD	34	↓	SPME – GC-MS
Phenole	Gaida <i>et al</i> ⁶²	COPD	190	↑	GC-MS
2-butylcyclohexanol	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↓	GC-MS

Ethanol	Schnabel <i>et al</i> ¹⁰⁷	Ventilator associated pneumonia	100	↑	GC-ToF-MS
Isopropyl Alcohol	Schnabel <i>et al</i> ¹⁰⁷	Ventilator associated pneumonia	100	↓	GC-ToF-MS
Benzyl alcohol	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↑	GC-MS
1-propanol	Schleich <i>et al</i> ⁶³	Asthma	521	↓	GC-MS
1-propanol	Van Oort <i>et al</i> ⁷⁴	Pneumonia	93	↑	GC-MS
Phenol derivatives					
Butylated hydroxytoluene	Cazzola <i>et al</i> ¹¹²	COPD	34	↓	SPME – GC-MS
m/p-Cresol,	Gaida <i>et al</i> ⁶²	COPD	190	—	GC-MS
Sulphides					
Phthalic anhydride	Phillips <i>et al</i> ²⁰	COPD	182	—	GC-MS
Sulphur dioxide	Phillips <i>et al</i> ²⁰	COPD	182	—	GC-MS
dimethyl disulfide	Pizzini <i>et al</i> ⁶¹	COPD	54	—	TD-GC-ToF-MS
methyl propyl sulfide	Pizzini <i>et al</i> ⁶¹	COPD	54	↑	TD-GC-ToF-MS
Permanent gases					
Ethyl 4-nitrobenzoate	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↓	GC-MS
Indole	Martinez <i>et al</i> ¹⁰⁹	COPD	61	↑	GC-IMS
Indole	Gaida <i>et al</i> ⁶²	COPD	190	—	GC-MS
Heterocycles					
Oxirane-dodecyl	Basanta <i>et al</i> ⁶⁷	COPD	71	—	GC-TOF-MS

γ -hydroxy-L-homoarginine	Bregy <i>et al</i> ⁶⁰	COPD	36	↑	SESI-MS
Nitriles					
Ace-tonitrile - C ₂ H ₃ N	Brinkman <i>et al</i> ¹⁰⁴	Asthma	23	↑	GC-MS
Hexyl ethylphosphonofluoridate	Cazzola <i>et al</i> ¹¹⁴	COPD	34	↓	SPME – GC-MS
Furans					
2-pentylfuran	Basanta <i>et al</i> ⁶⁷	COPD	71	↑	GC-Tof-MS
Tetrahydro-Furan	Schnabel <i>et al</i> ¹⁰⁷	Ventilator associated pneumonia	100	↓	GC-Tof-MS
Others					
2,6-Di-tert-butylquinone	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↓	GC-MS
3,4-Dihydroxybenzotrile	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↑	GC-MS
Allyl methyl sulphide	Ibrahim <i>et al</i> ¹⁰⁶	Asthma	58	↑	GC-MS
2'-Aminoacetophenone	Scott Thomas <i>et al</i> ⁸⁵	Cystic Fibrosis	46	↑	SPME – (GCMS)
Hexafluoroisopropanol	Van Oort <i>et al</i> ⁷⁴	Pneumonia	93	↓	GC-MS – compound considered by authors to be likely exogenous in origin

Table2: Summary of VOC biomarkers in various respiratory conditions from key breath studies and their reported concentration changes.

Additional References

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