



What molecules can be detected with SUPER SESI?

To answer this question, we have compiled a list with all molecules that have been reported by scientists using SESI.

There are several publications where the molecule identity is not reported. Some report peaks (m/z), others report molecular formulas.

For a molecule to be listed here, it must meet the following criteria:

- Based on SESI-MS spectra, a scientist has been able to identify the molecule and assign it to the corresponding peaks in the spectra.
- The identification must have been published in a peer-review journal.

This list includes only the molecules for which the author(s) provided MS data, molecular formula and a complete identification. The list also provides the molar mass of the molecules, the sample where the molecule was detected, the methods used to identify it, the details of the publication where it was first reported, and the year of publication.

Different identification processes have been implemented in different studies. In some studies, detectability was checked by evaporating a known standard and verifying that the expected peaks appear in the spectra. More comprehensive breath biomarker identification studies start by analyzing breath in real time with SESI-MS and SESI-MS/MS, and then verify the identification by analyzing the condensate with LC-MS/MS.

Take a look at the table, see what metabolites and molecules have been reported by other researchers and find if Super SESI can be helpful for your research.

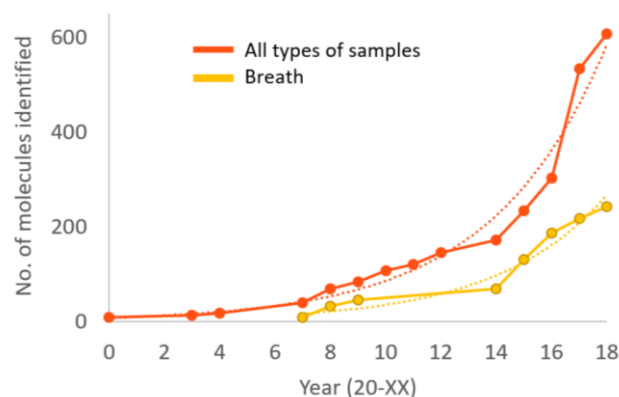
SESI is a rather new technique, that became available only recently. The samples studied with it include drugs of abuse, explosives, breath, volatiles of plants, yeast, and some bacterial cultures.

The total number of species identified (607) is a small fraction of all that can be detected. For instance, in breath samples, while a Super SESI - Q-Exactive detects 10.000 peaks in an exhalation*, only 242 species (2.4%) have been identified and reported.

(* See App. Note: Evaluation of No. Of detected species).

This gap shows that there is a lot to be discovered and understood.

The number of molecules identified with SESI is low, but it is accelerating, showing that the field is expanding in its infancy.



Only 2% of peaks detectable in breath have been identified. This large gap between the number of detectable peaks and the number of identified peaks shows that there is a lot of work to be done.

Bridging the information to knowledge gap is a challenge for researchers deciphering the volatilome.

FIT's mission is to enable scientists with the tools required to address this challenge.

molecule	molar mass	sample type	detector	identification method	publication title	DOI	year
amphetamine	135.21	evaporated	IMS-QMS	molecule known	Secondary Electrospray	10.1021/a	2000
methamphetamine	149.24	from liquid		before injection	Ionization Ion Mobility	c9907235	
Phencyclidine	243.39	sample			Spectrometry/Mass		
morphine	285.34				Spectrometry of Illicit		
cocaine	303.35				Drugs		
Tetrahydrocannabinol	314.47						
Lysergic acid diethylamide	323.44						
heroin	369.41						
dimethyl methylphosphonate (DMMP)	124.08	evaporated	IMS-	molecule known	Secondary Ionization of	10.1021/a	2003
pinacolyl methylphosphonate (PMP)	180.18	from liquid	ToFMS	before injection	Chemical Warfare Agent	c034349r	
diethyl phosphoramidate (DEPA)	153.12	sample			Simulants: Atmospheric		
2-(butylamino)ethanethiol (BAET)	133.26				Pressure Ion Mobility		
2-chloroethyl ethylsulfide (CEES)	124.63				Time-of-Flight Mass		
trinitrotoluene (TNT),	227.13	evaporated	IMS-QMS	molecule known	Secondary Electrospray	10.1021/a	2004
cyclo-1,3,5-trimethylene-2,4,6-trinitramine (RDX),	222.12	from liquid		before injection	Ionization-Ion Mobility	c0354591	
nitroglycerin (NG)	227.09	sample			Spectrometry for		
pentaerythritol tetranitrate (PETN)	316.14				Explosive Vapor		
Urea	60.06	breath	QQQ	MS-MS	Electrospray ionization	10.1016/j.	2007
triethylamine	353.68	evaporated	(MS)	molecule known	of volatiles in breath	jms.2007.0	
1-pyrroline	69.11	breath		MS-MS		5.008	
pyridine	79.10						
1-aminopropan-2-ol	75.11						
cysteamine	77.15						
4-aminobutanol	87.12						
isobutyl-3-methoxy-pyrazine	166.22	headspace of fresh fruit	Q-ToF	MS-MS	Differentiation of Maturity and Quality of Fruit Using Noninvasive Extractive Electrospray Ionization Quadrupole Time-of-Flight Mass	10.1021/a	
						c061843x	
Trimethylamine	59.11	headspace of fish meat at different stages of spoilage	Q-ToF	MS-MS, fragmentation pattern compared with reference standards	Neutral desorption sampling coupled to extractive electrospray ionization mass spectrometry for rapid differentiation of biosamples by metabolomic fingerprinting	10.1002/j	
Dimethylacetylamine	73.14					ms.1282	
N-Methylpyrrolidine	99.13						
N-Methylcyanoamide	56.07						
Putrescine	88.15						
Cadaverine	102.18						
Histamine	111.15						
Amino-2-hydroxycyclopentane	113.11						
Tyramine	137.18						
Spermidine	145.25						
Tryptamine	160.22						
Spermine	202.34						
Pentanethiol	104.22						
nicotine	162.23	in-vivo neutral desorption from	Q-ToF	MS-MS, fragmentation	Neutral Desorption Sampling of Living	10.1002/a	
caffeine	194.19					nie.20070	

molecule	molar mass	sample type	detector	identification method	publication title	DOI	year
phenylethylamine	121.18	headspace of reaction flask	Q-ToF	molecule known	Real-time, on-line monitoring of organic chemical reactions using extractive electrospray ionization tandem mass	10.1002/rc	2008
phenylethyl aminopropionitrile	150.17			before injection		m.3700	
3-[(2-cyanoethyl)phenylethylamino]propionitrile	174.24						
acetic anhydride	102.09						
benzyl acetate	150.18						
pyruvic acid	88.06	Breath	Q-ToF	MS-MS and CID database	Direct Analysis of Fatty Acid Vapors in Breath by Electrospray Ionization and Atmospheric Pressure Ionization-Mass Spectrometry	10.1021/a	
lactic acid	90.08					c801185e	
4-ketohexanoic acid	130.14						
propionic acid (C3)	74.08						
butiric (butanoic) acid (C4)	88.11						
valeric (pentanoic) acid	102.13						
caproic (hexanoic) acid	116.16						
heptanoic acid	130.18						
caprilic (octanoic) acid	144.21						
nonanoic acid	158.23						
capric (decanoic) acid	172.26						
undecanoic acid	186.29						
lauric (dodecanoic) acid	200.32						
tridecanoic acid	214.35						
Myristic (tetradecanoic) acid	228.37						
benzoic acid	122.12						
butanal	72.11						
3-methylbut-2-enal	84.12						
3-hexenal	98.14						
4-methylpentanal	100.16						
heptanal	114.18						
2-hydroxyhexanoic acid	132.16						
2-hydroxyheptanoic acid	146.18						
2-hydroxyoctanoic acid	160.21						
pentadecanoic acid	242.40	in-vivo neutral desorption from human skin	Q-ToF	MS-MS and CID database	On-line Detection of Human Skin Vapors	10.1016/j.	2009
palmitic (hexadecanoic) acid	256.43					asms.200	
dodecenoic acid	198.30					9.01.012	
Myristelaidic (tetradecenoic) acid	226.35						
pentadecenoic acid	240.38						
hexadecenoic acid	254.41						
heptadecenoic acid	268.40						
oleic (octadecenoic) acid	282.47						
pyruvaldehyde	72.06						
glyoxylic acid	74.04						
4-hydroxybutanoic acid	104.10						
3-methyl-2-oxobutanoic acid	116.11						
3-hydroxypentanoic acid	118.13						
alpha-Ketoisocaproic (4-methyl-2oxopentanoic) acid	130.14						

molecule	molar mass	sample type	detector	identification method	publication title	DOI	year						
phosphoric acid	97.99	headspace of beer samples	Linear Qtrap	MS ⁿ	Simultaneous sampling of volatile and non-volatile analytes in beer for fast fingerprinting by extractive electrospray ionization mass spectrometry	10.1007/s00216-010-3945-8	2010						
aspartic acid	133.11												
serine	105.09												
proline	115.13												
alanine	89.09												
threonine	119.12												
ethyl acetate	88.11												
isoamyl acetate	130.19												
Acetonitrile	41.05												
Ethanol	46.07												
Butanol	74.10	headspace of bacterial cultures	QQQ (MS)	MS-MS and CID database	Fast Detection of Volatile Organic Compounds from Bacterial Cultures by Secondary Electrospray Ionization-Mass Spectrometry	10.1128/JCM.00392-10							
Acetone	58.08												
Ethylene glycol	62.07												
Isopentanol	88.15												
Pyrimidine	80.09												
2-Pentanone	86.13												
4-Methylphenol	122.16												
Indole	117.15												
2-Aminoacetophenone	135.16												
2-Nonanone	128.21												
Methyl decanoate	186.29												
Octan-3-one	128.21							evaporated from liquid sample	QQQ (MS)	molecule known before injection	Optimisation of secondary electrospray ionisation (SESI) for the trace determination of	10.1039/b918899a	
2-Ethylhexanoic acid	144.21												
2,3-Butanediol	90.12												
Fentanyl	336.47							evaporated from liquid sample	Several MS configurations	molecule known before injection	Evaluation of extractive electrospray ionization and atmospheric pressure chemical	10.1016/j.jms.2010.10.011	2011
Sulfentanyl	386.55												
Naloxone	327.27												
Norfentanyl	232.32												
gamma-hydroxybutyrolactone	86.09	evaporated from liquid sample	Several MS configurations	molecule known before injection	Evaluation of extractive electrospray ionization and atmospheric pressure chemical ionization for the detection of narcotics in	10.1255/ejms.1146							
1-Butylamine	73.14												
1-Pentylamine	87.16												
1-Hexylamine	101.19												
1-Heptylamine	115.22												
1-Octylamine	129.24												
1-Nonylamine	143.27												
1-Decylamine	157.30												
4-hydroxy-Valproic Acid-g-lactone	142.10							Breath	QToF	MS/MS	Real-time, in vivo monitoring and pharmacokinetics of valproic acid via a novel biomarker in exhaled breath	10.1039/c1cc10343a	

molecule	molar mass	sample type	detector	identification method	publication title	DOI	year
Ethylamine	45.08	evaporated from liquid sample	IMS-QToF	molecule known before injection	Mechanistic Study on the Ionization of Trace Gases by an Electrospray Plume	10.1016/j.jms.2011.12.010	2012
Dimethylamine	45.08						
Diethylamine	73.14						
Triethylamine	101.19						
Dibutylamine	129.24						
Trihexylamine	269.50						
Atenolol	266.34	evaporated from liquid	Ion Trap	MS ⁿ	Sensitive detection of drug vapors using an ion funnel interface for secondary electrospray ionization mass spectrometry	10.1002/jms.2982	
Salbutamol	239.31						
1-Propanol	60.09						
2-Pentanol	88.15						
1-Hexanol	102.16						
Eugenol	164.20						
Hexanal	100.16						
Octanal	128.21						
Geraniol	154.25						
Citronellol	156.27						
Decanal	156.20						
Undecanal	170.29						
Dodecanal	184.32						
Citronellyl acetate	198.30						
Tetradecanal	254.41						
Pentadecanal	226.40						
Hexadecanal	240.42						
alfa-Bisabolol	284.70						
Ethyl linoleate	308.50						
gamma-butyrolactone	86.09	headspace of drinks, saliva and urine	Ion Trap	molecule known before injection	In situ detection of γ-hydroxybutyrate and γ-butyrolactone in drinks by secondary electrospray ionization	10.1039/C2AY26009C	2013

molecule	molar mass	sample type	detector	identification method	publication title	DOI	year						
12-Amino-dodecanoic acid	215.33	Breath	LTQ-Orbitrap	HRMS followed by HRMS-MS and LCMSMS	A new strategy based on real-time secondary electrospray ionization and high-resolution mass spectrometry to discriminate endogenous and exogenous compounds in exhaled breath	10.1007/s11306-013-0568-z	2014						
Evocarpine	122.12												
Capnine	351.50												
Dioctyl phthalate	390.56												
Glyceric acid	106.08												
Erythronic acid	136.10												
Ribose	150.13												
Benzylazanium/o-toluidine/N-methyl-aniline	107.16												
N-Butylaniline/phentermine/2,6-diethylaniline	149.23												
3 Hexylpyridine	93.13												
But-2-enoic acid	86.09												
trans-2-Octenoic acid	142.20												
4-Hydroxynonenal	156.23												
Methyl jasmonate	224.30												
3-oxo-2-pentyl-cyclopentanebutanoic acid	240.34												
Morpholine	87.10												
2,5-Dihydro-2,4,5-trimethyloxazole	113.16												
(S)-Oleuropeic acid	184.23												
1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1 / 6-heptadien	110.20												
3-Methyl-alpha-ionyl acetate	250.38												
diethyl ethylphosphonate (DEEP)	166.16	Headspace of cell culture plates	QToF	HRMS and isotopic patterns	Fingerprinting Breast Cancer vs. Normal Mammary Cells by Mass Spectrometric Analysis of Volatiles	10.1038/sr ep05196							
Diisopropyl methylphosphonate (DIMP)	180.18												
malathion	330.36												
dichlorvos (DCV)	220.97												
phoxim (PHX)	298.30												
thiodiglycol (TDG)	122.19												
2-nonenal	140.22	evaporated from liquid sample	Ion Trap	molecule known before injection	Direct Quantification of Chemical Warfare Agents and Related Compounds at Low ppt Levels: Comparing Active Capillary Dielectric	10.1021/a c5035874							
2-decenal	154.25												
2-undecenal	168.28												
2-dodecenal	182.3												
2-tridecenal	196.33												
2-tetradecenal	210.36												
4-hydroxy-2-hexenal	114.14												
4-hydroxy-2-heptenal	128.17												
4-hydroxy-2-octenal	142.20												
4-hydroxy-2-decenal	170.25												
4-hydroxy-2-undecenal	184.28												
4-hydroxy-2-dodecenal	198.30												
4-hydroxy-2-tridecenal	212.33												
4-hydroxy-2-tetradecenal	226.36												
4-hydroxy-2-pentadecenal	240.38												
4-hydroxy-2-hexadecenal	254.41												
4-hydroxy-2,6-heptadienal	126.16												
4-hydroxy-2,6-octadienal	140.18												
4-hydroxy-2,6-nonadienal	154.21												
4-hydroxy-2,6-decadienal	168.24												
4-hydroxy-2,6-undecadienal	182.26												
4-hydroxy-2,6-dodecadienal	196.29												
4-hydroxy-2,6-tridecadienal	210.32												
4-hydroxy-2,6-tetradecadienal	224.34												
4-hydroxy-2,6-pentadecadienal	238.37	in-vivo headspace of mouse cage	QToF	MS/MS	Drug Pharmacokinetics Determined by Real-Time Analysis of Mouse Breath	10.1002/a nie.20150 3312							
Ketamine	237.73												
Norketamine	223.70												
hydroxyketamine	253.73												
hydroxynorketamine	239.70												
dehydronorketamine	221.68												
propofol	178.27												
Valproic acid	144.21												
methylfuran	82.10							Breath	HRMS Orbitrap	HRMS followed by HRMS-MS and LCMSMS	Real-Time High-Resolution Tandem Mass Spectrometry Identifies Furan Derivatives in Exhaled Breath	10.1021/a cs.analch em.5b015 09	
ethylfuran	96.13												
propylfuran	110.16												
butylfuran	124.18												
pentylfuran	138.21												
hexylfuran	196.24												
heptylfuran	166.26												
octylfuran	180.29												
nonylfuran	194.31												
decylfuran	208.34												
undecylfuran	222.37												
dodecylfuran	236.39												
formylfuran	97.09												
acetyl furan	110.12												
acetonefuran	126.15												
hydroxymethyl furan	98.10	Breath	QToF	HRMS followed by HRMS-MS and LC-MS/MS	Detection and Quantification of Benzothiazoles in Exhaled Breath and Exhaled Breath Condensate by Real-	10.1021/a cs.est.5b0 3809							
benzothiazole	135.19												
2-aminobenzothiazole	150.20												
2-mercaptobenzothiazole	167.25												
2-hydroxybenzothiazole	151.19												
2-methylthiobenzothiazole	181.30												
2-(4-35 morpholinyl)benzothiazole	220.07	evaporated from liquid sample	QToF	molecule known before injection	Vapor Pressure of Hexamethylene Triperoxide Diamine (HMTD) Estimated Using Secondary Electrospray Ionization Mass Spectrometry	10.1021/a cs.jpca.5b 08929							
hexamethylene triperoxide diamine	208.17												
Isoprene	68.12							Breath	QToF	MS/MS	The Effect of CPAP Withdrawal on Exhaled Breath in Obstructive Sleep Apnea – A Randomized Controlled Trial	10.1136/th oraxjnl- 2015- 207597	
2-pentenal	84.12												
Methylphenol	324.40												
Homocysteine thiolactone	117.17												
Ethylphenol	122.16												
Mevalonic acid	148.16												
Digitaiose	178.18												

molecule	molar mass	sample type	detector	identification method	publication title	DOI	year						
Melatonin	232.28	evaporated from liquid sample	HRMS Orbitrap	molecule known before injection	Numerical Modeling and Experimental Validation of a Universal Secondary Electrospray Ionization	10.1016/j.snb.2015.09.073	2016						
Acetaminophen	151.16	in-vivo air in plant cage	HRMS Orbitrap	HRMS (MS & MS/MS)	Capturing in Vivo Plant Metabolism by Real-Time Analysis of Low to High Molecular Weight Volatiles	10.1021/a cs.analchem.5b04452							
Pentobarbital	226.27												
Midazolam	325.78												
β -caryophyllene	204.36												
3-hexenyl acetate	142.20												
monoterpene	136.23												
sesquiterpene	204.36												
hexenol	100.16												
methyl salicylate	152.15												
monoterpene alcohol	152.23												
hexenyl butyrate	170.25												
4,8-dimethylnona-1,3,7-triene (DMNT)	150.26												
4,8,12-trimethyltrideca-1,3,7,11-tetraene (TMTT)	218.38												
monothiophene	98.17												
myosmine	146.19							direct ecigarrete puff	HRMS Orbitrap	HRMS (MS & MS/MS)	Real-Time Chemical Analysis of E-Cigarette Aerosols By Means Of Secondary Electrospray	10.1002/c hem.2015.04450	
Acetyl Pyrazine	122.12							Breath	HRMS Orbitrap	HRMS (MS & MS/MS)	Expanding metabolite coverage of real-time breath analysis by coupling a universal secondary electrospray ionization source and high resolution mass spectrometry - A pilot study on tobacco smokers	10.1088/1752-7155/10/1/016010	
Ethylmalto	140.14												
Isoamyl isovalerate	172.26												
4-hydroxy-2-pentenal	100.11												
4-hydroxy-2,6-pentadienal	98.10												
4-hydroxy-2,6-hexadienal	112.13												
hexenoic acid	114.14												
heptenoic acid	128.17												
nonenoic acid	156.22												
decenoic acid	170.25												
undecylenic acid	184.27												
tridecylenic acid	212.32												
pentadecylenic acid	240.38												
oxopentanoic acid	116.12												
oxoheptanoic acid	144.17												
oxononanoic acid	172.22												
oxooctenoic acid	186.25												
oxononenoic acid	200.28												
oxodecenoic acid	214.30												
heptenedioic acid	184.10	Breath	HRMS Orbitrap	HRMS (MS & MS/MS followed by HPLC-MS-MS)	Secondary electrospray ionization coupled to high-resolution mass spectrometry reveals tryptophan pathway metabolites in exhaled human breath	10.1039/C6CC03070J							
Anthranilate	137.14												
4,8-Dihydroxyquinoline	161.16												
4,6-Dihydroxyquinoline	161.16												
3-Methylindole	163.17												
Indole-3-acetate	175.18												
5-Hydroxyindoleacetaldehyde	175.18												
3-Hydroxykynurenamine	180.20												
5-Methoxyindoleacetate	205.21												
4-(2-Aminophenyl)-2,4-dioxobutanoate	207.18												
L-Kynurenine	208.22												
N-Acetylserotonin	218.25												
5-Hydroxy-L-tryptophan	220.23												
4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate	223.05												
5-Hydroxykynurenine	224.21												
N-Formylkynurenine	236.22												
6-Hydroxymelatonin	248.28												
Formyl-N-acetyl-5-methoxykynurenamine	236.27												
Ornithine	132.16							Breath	HRMS Orbitrap	HRMS (MS & MS/MS followed by HPLC-MS-MS)	Real-Time Quantification of Amino Acids in the Exhalome by Secondary Electrospray Ionization-Mass Spectrometry: A Proof-of-	10.1373/clinchem.2016.256909	
Glycine	75.07												
Valine	117.15												
Iso-leucine	131.17												
Phenylalanine	165.19												
Lysine	146.19												
sulfate/sulfuric acid	98.08	Breath	HRMS Orbitrap	HRMS and isotopic patterns	Direct human breath analysis by secondary nano-ESI ultra-high resolution mass spectrometry: Importance of high mass resolution and mass	10.1002/rcm.7794							
silicate/silicic acid	96.11												
nitrate/nitric acid	63.01												
dichlorobenzene	147.01												
polysiloxane (n=6)/Dodecamethylcyclohexasiloxane	444.92												
sulfosuccinate/sulfosuccinic acid	198.15												
monoacylglycerol	330.50												

molecule	molar mass	sample type	detector	identification method	publication title	DOI	year						
acetic acid	60.05	Headspace of fresh fruits	HRMS Orbitrap	HRMS, isotopic patterns	Rapid fingerprinting of grape volatile composition using secondary electrospray	10.1016/j.foodcont.2017.04.041	2017						
β -ionone	192.30												
(E)-2,4-heptadienal	110.15												
4-vinylphenol	120.15												
2,4-dinitrotoluene (DNT)	182.13	Air surrounding canine training samples	QQQ (MS)	molecule known before injection	Direct Quantification of Chemical Warfare Agents and Related Compounds at Low ppt	10.1021/a cs.analchem.7b00451							
2,6-dinitrotoluene (DNT)	182.13												
triacetone triperoxide (TATP)	222.24												
cyclohexanone	98.15	lab ambient air	HRMS Orbitrap	HRMS, MS/MS & isotopic patterns	Secondary electrospray ionization proceeds: Via gas-phase chemical	10.1039/C7AY01121K							
phthalic anhydride	148.10												
Dibutylphthalate	278.34												
2,2,2-trifluoroethanol	100.04												
ω -hydroxynonanoic acid	174.24							Breath	QToF	HRMS (MS & MS/MS followed by HPLC-MS-MS)	Mass-Spectrometric Detection of Omega-Oxidation Products of Aliphatic Fatty Acids in Exhaled Breath	10.1021/a cs.analchem.7b02092	
ω -hydroxydecanoic acid	188.26												
ω -hydroxyundecanoic acid	202.29												
ω -hydroxydodecanoic acid	216.32												
ω -hydroxytridecanoic acid	230.34												
ω -hydroxytetradecanoic acid	244.37												
ω -hydroxypentadecanoic acid	258.40												
ω -oxodecanoic acid	186.25												
ω -oxotridecanoic acid	228.33												

molecule	molar mass	sample type	detector	identification method	publication title	DOI	year
ω-oxotetradecanoic acid	242.35						2017
ω-oxopentadecanoic acid	256.38						
pentanedioic acid	132.11						
hexanedioic acid	146.14						
heptanedioic acid	160.17						
octanedioic acid	174.19						
nonanedioic acid	188.22						
decanedioic acid	202.25						
undecanedioic acid	216.27						
docecanedioic acid	230.30						
tridecanedioic acid	244.33						
tetradecanedioic acid	258.35						
pentadecanedioic acid	272.38						
salbutamol-4-O-sulfate	319.38	Breath	QToF	HRMS (MS & MS/MS)	Metabolic effects of	10.1088/1	
formoterol	344.41			followed by HPLC-	inhaled salbutamol	752-	
Methyl cinnamate	162.19	headspace of	HRMS	HRMS, Isotopic	Comprehensive Real-	10.1038/s	
Benzofuran	118.10	in-vivo yeast	Orbitrap	labeled molecular	Time Analysis of the	41598-017-	
1-Methylpyrrolo[1,2-a]pyrazine	132.78	culture fed with		formula compared	Yeast Volatilome	14554-y	
Vanillic acid	168.14	isotopically		with metabolomic			
Coixinden A	190.19	labeled		database			
Diatretin 2	145.11	glucose					
Indoleacrylic acid	187.19						
4-Amino-2-methyl-1-naphthol	173.21						
PHENYL 2-PYRIDYL KETONE	183.21						
Ricinine	164.16						
Vanillin	152.15						
4-hydroxy-3-nitrophenylacetate	197.14						
Oroselone	226.23						
Resveratrol	228.25						
(3-Methyl-2-butenyl)-benzene	146.23						
3-Propylidene-1(3H)-isobenzofuranone	174.20						
3-(indol-3-yl)pyruvic acid	203.19						
Dracunculol	220.18						
2-Heptanone	114.18						
Cyclohexane	84.16						
α-Amylcinnamyl isovalerate	288.42						
Nerol	154.25						
Ethyl vanillin	166.17						
Alpha-Ketoisovaleric acid	116.12						
2-Undecanone	170.29						
xi-1-Butoxy-1-methoxyethane	132.20						
isobutanol	74.12						
Ethyl decanoate	200.32						
Cyclopentane	70.10						
Hexanediol	118.17						
4-Hydroxymethylpyrazole	98.10						
Pyrrolidine	71.12						
(Z)-9-Cycloheptadecen-1-one	250.42						
Stearidonic acid	276.41						
Isopentyl hexanoate	186.29						
Ethyl octanoate	172.26						
Propyl decanoate	214.34						
Octanedioic acid / dihexyl ester	342.51						
Octadecanedioic acid	314.46						
Octanoic acid	144.21						
Ethyl 9-hexadecenoate	282.46						
1-Phenylheptane	176.30						
α-Curcumenol	202.33						
Butylated hydroxytoluene	220.35						
1-octen-3-one	126.20						
2-Isopropyl-1,4-hexadiene	124.22						
1,3-Octadiene	110.20						
3-Methylcyclopentene	82.14						
Benzene	78.11						
Toluene	92.14						
1,3-Diisopropylbenzene	162.27						
1-Methyl-1,3-cyclohexadiene	94.15						
(Z)-1,3-Octadiene	108.18						
Ethylbenzene	106.16						
β-Farnesene	204.35						
1-Methyl-4-(1-methylpropyl)-benzene	148.24						
Cumene	120.19						
Nerolidol	222.37						
Santene	122.21						
p-Cymene	134.22						
Acetamide	59.07						
Cyclopentadiene	66.10						
Quinaldic acid	173.17						
1-nitrosonaphthalene	157.17						
Myrcene	136.23						
Vinyl caffeate	206.19						
4-Methylacetophenone	134.17						
Syringol	154.16						
Tyrosol	138.16						
2-Furanmethanol	98.10						
2-Acetylactate	132.11						
Trihydroxybutane	106.12						
3-Dehydroxycarnitine	145.20						
2,4-Dimethyl-2-pentene	98.19						
Geranyl valerate	238.36						

These compounds are all listed in the same publication of 2017

Dihydrofarnesol	224.38
(S)-3,7-Dimethyl-1,6-octadiene	138.25
2-Methylisoborneol	168.28
2,6-Dimethyl-naphtalene	156.22
1-Acetyl-2-methylcyclopentene	192.34
α-Methylstyrene	118.18
2-methoxyphenol	76.10
Methyl tetradecanoate	242.40
4-Methyl-2-methylene-1-(1-methylethylidene)-cyclohexane	150.26
(Z)-1,5-Tridecadiene	180.33
Propyl hexanoate	158.24
trans,trans-2,4-decadienal	152.23
3-Methyl-4-octanolide	156.22
β-Calacorene	200.32
1,3-Butadiene	54.09
1-(1-methylethenyl)-3-(1-methylethyl)-benzene	160.25
Serratol	290.48
Cembrene	272.47
Geranic acid	168.23
2,5-Dimethyl-4-ethoxy-3(2H)-furanone	156.18
Carvone	150.22
Ethyl pentanoate	130.18
Furaneol	128.13
Pyridoxal	167.16
5-Hydroxydopamine	169.18
Ambronide	236.39
Zingerone	194.23
Lavander lactone	126.15
Isomyristicin	192.21
Glycerol	92.09
Ethyl hexadecanoate	284.48
3,7-Dimethyl-1,5-octadien-3,7-diol	170.25
Methyl succinate	128.17
2-nonanone	142.24
4-Methylcyclohexanone	112.17
Dehydro-p-cymene	132.20
Ethyl 9-decenoate	198.30
Sorbic acid	112.13
2,4-Dimethyl-5-propyloxazole	139.19
Ethyl geranyl acetone	208.34
Phenylethyl acetate	164.20
Hexa-2,4-dienol	98.14
Dendrolasin	218.33
Isogermafurene	216.32
2-Methyl-4-phenyl-2-butanol	164.24
1-Methyl-4-(1-methyl-2-propenyl)-benzene	174.28
Dihydroactinidiolide	180.24
Dihydroeugenol	166.22
1,4-Isopneadiol	170.21
Cyperotundone	216.36
2-Amino-2-methyl-1,3-propanediol	105.14
3-ethoxy-1-propanol	104.15
Ethyl 4-hydroxybutanoate	132.16
Ethyl 2-hydroxy propanoate	118.13
2,3-pentanedione	100.12
(R)-Acetoin	88.10
Norfuraneol	114.10
propylene glycol	76.09
Propanal	58.08
Capsidiol	236.35
1-Ethyl-3,5-diisopropyl-benzene	190.32
2-phenylbut-2-enal	146.19
2,6-Di-tert-butyl-4-ethylphenol	234.38
7Z,10Z-Hexadecadienoic acid	252.39
2-Methylbutanal	86.13
Phenol	94.11
Anethole	148.20
2-Isopropylfuran	110.15

Continues

Continues

These compounds are all listed in the same publication of 2017

Ethyl 2-hexenoate	142.20
3-Oxoocanoic acid	158.19
6-Methyl-3,5-heptadiene-2-one	124.18
m-Cresol	108.14
Anapear	154.21
4-Isopropylphenylacetaldehyde	162.23
4-Ethyl-2-methoxyphenol	152.19
Procurcumenol	234.33
Benzenepropanol	136.19
Homovanillyl alcohol	168.19
Costunolide	232.32
3-Methoxybenzenepropanoic acid	180.20
Isoamyl 2-furoate	182.22
Paulinic acid	310.51
Linoleic acid	280.44
1-Octen-3-ol	128.21
4-Vinylguaiaicol	150.17
Succinic anhydride	100.07
Cycloserine	102.09
4-Hydroperoxy-2-nonenal	172.22
Geranyl acetone	194.31
Homodihydrojasmon	180.29
Ethyl lactate	114.14
Propyl acetate	102.13
Ethyl formate	74.08
Cyclopentanone	84.12
Ethoxy ethene	72.11
Methyleugenol	178.23
Dihydromyoporone	252.35
Neryl formate	182.26
3-Buten-2-one	70.09
Valerenolic acid	250.33
4,11,13,15-Tetrahydroindolizidine B	268.35
(±)-(Z)-2-(5-Tetradecenyl)cyclobutanone	264.44
Sinapyl alcohol	210.23
4-Pyridoxic acid	183.16
α-Isomethyl-ionone	206.32
1,1,6-Trimethyl-1,2-dihydronaphthalene	172.27
Hexyl 2-furoate	196.24
Humulinic acid A	266.33
Ethylene brassylate	270.36
L-Octanoyl carnitine	287.39
Dihydrogeranylacetone	196.33
γ-Undecalactone	184.27
Citronellyl propionate	212.33
8-Heptadecenal	252.43
Citral	152.24
Butanoic acid	88.11
ethylhexanoate	144.21
diacetyl	86.09
2-phenyl ethanol	122.16
nona-2,6-dienal	138.21

molecule	molar mass	sample type	detector	identification method	publication title	DOI	year
2-Hydroxyisobutyric acid	104.11	Breath	QToF	UHPLC-HRMS of EBC	Real-time mass spectrometric identification of metabolites characteristic of Chronic Obstructive Pulmonary	10.1016/j.clinms.2018.02.003	2018
Aceto hydroxybutanoic acid	146.14						
(+)-g-hydroxy-L homoarginine	204.23	Breath	QToF	UHPLC-HRMS of EBC	Real-Time exhaled breath analysis in patients with cystic fibrosis and controls	10.1088/1752-7163/aab7fd	
Oxo-tetradecenoic acid	240.34						
Hexadecatrienoic acid	250.38	Breath	QToF	UHPLC-HRMS of EBC	Real-Time Monitoring of Tricarboxylic Acid Metabolites in Exhaled	10.1021/aacs.analchem.7b046	
2-oxoglutaric acid semialdehyde	160.12						
Docosahexanoic acid	328.49	Breath	HRMS Orbitrap	HRMS (MS & MS/MS) followed by HPLC-MS-MS)	Differentiating antibiotic-resistant Staphylococcus aureus using secondary electrospray ionization tandem mass spectrometry (SESI-	10.1021/aacs.analchem.8b03029	
Malate /malic acid	134.09						
Alpha-ketoglutarate / alpha-ketoglutaric acid	146.11	headspace of bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
cis-aconitate / cis-aconitic acid	174.11						
tryptophan	204.23	headspace of bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
asparagine	132.12						
tyrosine	181.19	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
oxalic acid	90.03						
formic acid	46.03	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
oxaloacetic acid	132.07						
octadecanoic acid	284.48	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
maleimide	97.07						
5-valerolactone	100.12	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
2-hydroxybutyric acid	104.10						
choline	104.17	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
hydroxypyruvate	104.06						
2-aminophenol	109.13	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
creatinine	113.12						
maleamate	115.09	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
5-aminopentanoate	117.15						
N-acetyl glycine	117.10	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
betaine	117.15						
guanidinoacetate	117.11	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
mesoxalate	174.15						
nicotinamide	122.12	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
3-Hydroxybenzaldehyde	122.12						
5-oxo-D-proline	129.11	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
pipecolate	129.16						
N-acetylputrescine	130.19	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
5-aminopentanoate	117.15						
N-acetyl glycine	117.10	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
betaine	117.15						
guanidinoacetate	117.11	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
mesoxalate	174.15						
nicotinamide	122.12	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
3-Hydroxybenzaldehyde	122.12						
5-oxo-D-proline	129.11	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
pipecolate	129.16						
N-acetylputrescine	130.19	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
5-aminolevulinic acid	131.13						
creatine	149.15	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
4-hydroxyproline	131.13						
3-ureidopropionate	132.12	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
mono-ethylmalonate	160.17						
oxalacetic acid	132.07	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
deoxyribose	134.13						
homocysteine	135.18	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
5-hydroxymethyluracil	142.11						
O-acetyl-L-serine	147.13	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
citramalate	148.11						
guanine	151.13	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
octopamine	153.18						
4-hydroxy-L-phenylglycine	167.16	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
noradrenaline	169.18						
S-carboxymethyl-L-cysteine	179.20	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
D-(+)-glucosamine	179.17						
O-phospho-DL-serine	185.07	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
D-glucuronic acid	194.14						
methyl beta-D-galactoside	194.18	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
ferulate	194.18						
N-acetyl-D-mannosamine	221.21	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
palmitoleic acid	254.41						
uracil	112.09	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
fumaric acid	116.07						
succinic acid	118.09	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
ascorbate	198.11						
petroselinic acid	282.50	headspace of gut bacterial cultures	QQQ	MS/MS	Headspace Gas Monitoring of Gut Microbiota Using Targeted and Globally Optimized Targeted Secondary Electrospray Ionization Mass Spectrometry	10.1021/aacs.analchem.8b03517	
elaidic acid	282.46						
2-Nitrophenol	139.11	Breath	QToF	UHPLC-HRMS of EBC	Real-Time Breath Analysis Reveals Specific Metabolic Signatures of COPD Exacerbations	10.1016/j.cheest.2018.12.023	
4-Methyl-2-nitrophenol	153.14						
3-Hydroxy-2-nitrophenol	155.11	Breath	QToF	UHPLC-HRMS of EBC	Real-Time Breath Analysis Reveals Specific Metabolic Signatures of COPD Exacerbations	10.1016/j.cheest.2018.12.023	
4-Hydroxy-3-nitrobenzaldehyde	167.12						
Methoxy-nitrophenol	169.13	Breath	QToF	UHPLC-HRMS of EBC	Real-Time Breath Analysis Reveals Specific Metabolic Signatures of COPD Exacerbations	10.1016/j.cheest.2018.12.023	
Hydroxy-nitrobenzoic acid	183.12						
2-Nitro-tyrosol	183.16	Breath	QToF	UHPLC-HRMS of EBC	Real-Time Breath Analysis Reveals Specific Metabolic Signatures of COPD Exacerbations	10.1016/j.cheest.2018.12.023	
2,4-Dinitrophenol	184.11						
Nitrovanillin	197.14	Breath	QToF	UHPLC-HRMS of EBC	Real-Time Breath Analysis Reveals Specific Metabolic Signatures of COPD Exacerbations	10.1016/j.cheest.2018.12.023	
2-Methyl-4,6-dinitrophenol	198.13						
Allylsine	145.16	Breath	QToF	UHPLC-HRMS of EBC	Molecular breath analysis supports	10.1111/resp.13465	2019
Pyroglutamic acid	129.04						

This table is a constant work in progress. If you find a new molecule, please contact us and we will upgrade it with the corresponding reference.