SUPER SESI



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.

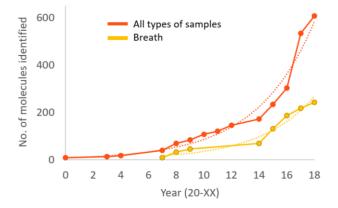
Take a look at the table, see what metabolites and molecules have been reported by other researchers and find if Super SESI can be helpful for your research.

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.

	molar						
molecule	mass	sample type		identification method	publication tittle	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.i	2007
trioctylamine	353.68	evaporated	(MS)	molecule known		jms.2007.0)
		from liquid		before injection		5.008	
1-pyrroline	69.11	breath		MS-MS			
pyridine	79.10						
1-aminopropan-2-ol	75.11						
cysteamine	77.15						
4-aminobutanal	87.12						
isobutyl-3-methoxypyrazine	166.22	headspace of	Q-ToF	MS-MS	Differentiation of	10.1021/a	
		fresh fruit			Maturity and Quality of Fruit Using Noninvasive Extractive Electrospray Ionization Quadrupole Time-of-Flight Mass	c061843x	
Trimethylamine	59.11	headspace of	Q-ToF	MS-MS,	Neutral desorption	10.1002/j	
Dimethylacetylamine	73.14	fish meat at		fragmentation	sampling coupled to	ms.1282	
N-Methylpyrolidine	99.13	different		pattern compared	extractive electrospray		
N-Methylcyanoamide	56.07	stages of		with reference	ionization mass		
Putrescine	88.15	spoilage		standards	spectrometry for rapid		
Cadaverine	102.18				differentiation of		
Histamine	111.15				biosamples by		
Amino-2-hydroxyclyclopentanone	113.11				metabolomic		
Tyramine	137.18				fingerprinting		
Spermidine	145.25						
Tryptamine	160.22						
Spermine	202.34						
Pentanethiol	104.22						
nicotine	162.23	in-vivo neutral	Q-ToF	MS-MS,	Neutral Desorption	10.1002/a	
caffeine	194.19	desoption from		fragmentation	Sampling of Living	nie.20070	

	molar							
molecule	mass	sample type	detector	identification method	publication tittle	DOI	year	
phenylethylamine	121.18	headspace of	Q-ToF	molecule known	Real-time, on-line	10.1002/rc	2008	
phenylethyl aminopropionitrile	150.17	reaction flask		before injection r	monitoring of organic	m.3700		
3-[(2-cyanoethyl)phenylethylamino]propionitrile	174.24				chemical reactions using			
acetic anhydride	102.09				extractive electrospray			
benzyl acetate	150.18				ionization tandem mass			
pyrubic acid	88.06	Breath	Q-Tof	MS-MS and CID	Direct Analysis of Fatty	10.1021/a		
lactic acid	90.08			database	Acid Vapors in Breath by	c801185e		
4-ketohexanoic acid	130.14				Electrospray Ionization			
propionic acid (C3)	74.08				and Atmospheric			
butiric (butanoic) acid (C4)	88.11				Pressure Ionization-			
valeric (pentanoic) acid	102.13				Mass Spectrometry			
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							
tricedanoic 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	1						
pentadecanoic acid	242.40	in-vivo neutral	Q-Tof	MS-MS and CID	On-line Detection of	10.1016/j.j	2009	
palmitic (hexadecanoic) acid	256.43	desoption from		database	Human Skin Vapors	asms.200		
dodecenoic acid	198.30	human skin				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							

Identified species. Page 1 of 6

	molar						
molecule	mass	sample type	detector	identification method	publication tittle	DOI	year
phosphoric acid	97.99	headspace of	Linear	MS ⁿ	Simultaneous sampling	10.1007/s	
aspartic acid	133.11	beer samples	Qtrap		of volatile and non-	00216-010-	
serine	105.09				volatile analytes in beer	3945-8	
proline	115.13				for fast fingerprinting by		
alanine	89.09				extractive electrospray		
threonine	119.12				ionization mass		
ethyl acetate	88.11				spectrometry		
isoamyl acetate	130 19						
Acetonitrile	41.05	headspace of	QQQ	MS-MS and CID	Fast Detection of	10.1128/JC	
Ethanol	41.05	bacterial	(MS)	database	Volatile Organic	M.00392-	
Butanol	74.10	cultures	(IVIS)	Galabase	Compounds from	10	
Acetone	58.08	cultures			Bacterial Cultures by	10	
Ethylene glycol	62.07				Secondary Electrospray		
Isopentanol	88.15				Ionization-Mass		
Pyrimidine	80.09				Spectrometry		
2-Pentanone	86.13				opectionicity		
4-Methylphenol	122.16						
Indole	117.15						
2-Aminoacetophenone	135.16						
2-Nonanone	128.21						
Methyl decanoate	186.29	evaporated	000	molecule known	Optimisation of	10.1039/b	
Octan-3-one	128.21	from liquid	(MS)	before injection	secondary electrospray	918899a	
2-Ethylhexanoic acid	144.21	sample			ionisation (SESI) for the		
2,3-Butanediol	90.12				trace determination of		
Fentanyl	336.47	evaporated	Several	molecule known	Evaluation of extractive	10.1016/j.i	2011
Sulfentanyl	386.55	from liquid	MS	before injection	electrospray ionization	jms.2010.1	
Naloxone	327.27	sample	configur		and atmospheric	0.011	
Norfentanyl	232.32		ations		pressure chemical		
gamma-hydroxybutyrolactone	86.09	evaporated	Several	molecule known	Evaluation of extractive		
		from liquid	MS	before injection	electrospray ionization		
		sample	configur		and atmospheric		
			ations		pressure chemical		
					ionization for the		
					detection of narcotics in		
1-Butylamine	73.14	evaporated	Ion Trap	molecule known	Contribution of liquid-	10.1255/ej	
1-Pentylamine	87.16	from liquid		before injection	phase and gas-phase	ms.1146	
1-Hexylamine	101.19	sample			ionization in extractive		
1-Heptylamine	115.22				electrospray ionization		
1-Octylamine					mass spectrometry of		
1-Nonylamine 1-Decvlamine	143.27 157.30				primary amines		
1-Decylamine 4-hydroxy–Valproic Acid–g-lactone	157.30	Breath	QToF	MS/MS	Real-time, in vivo	10.1039/c1	
+-nyuroxy=valproic Acid=g-lactone	142.10	breath	UIOF	IVI3/IVI3	monitoring and	10.1039/c1 cc10343a	
					pharmacokinetics of		
					valproic acid via a novel		
					biomarker in exhaled		
					breath		

	Compounds from Bacterial Cultures by Secondary Electrospray Ionization-Mass Spectrometry	10		
vn	Optimisation of	10.1039/b		

	molar						
molecule	mass	sample type	detector	identification method	•	DOI	yea
Ethylamine	45.08	evaporated	IMS-	molecule known	Mechanistic Study on the		
Dimethylamine	45.08	from liquid	QToF	before injection	Ionization of Trace	jms.2011.1	
Diethylamine	73.14	sample			Gases by an Electrospray	2.010	
Triethylamine	101.19				Plume		
Dibutylamine	129.24						
Trihexylamine	269.50						
Atenolol	266.34	evaporated from liquid	Ion Trap	MS ⁿ	Sensitive detection of	10.1002/j	
Salbutamol	239.31				drug vapors using an ion funnel interface for	ms.2982	
1-Propanol	60.09	in-vivo neutral					
2-Pentanol	88.15	desoption of fresh fruit headspace			secondary electrospray ionization mass		
1-Hexanol	102.16				spectrometry		
Eugenol	164.20				specificity		
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	Ion Trap	molecule known	In situ detection of y-	10.1039/C	2013
- ,		drinks, saliva		before injection	hydroxybutyrate and y-	2AY26009C	
		and urine			butyrolactone in drinks		
					by secondary		
					electrospray ionization		

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molecule	molar mass	sample type	detector	identification method	publication tittle	DOI	yea
12-Amino-dodecanoic acid	215.33	Breath	LTQ-	HRMS followed by	A new strategy based on	10.1007/s	201
Evocarpine	122.12		Orbitrap	HRMS-MS and	real-time secondary	11306-013-	
Capnine	351.50			LCMSMS	electrospray ionization	0568-z	
Dioctyl phtalate	390.56				and high-resolution		
Glyceric acid	106.08				mass spectrometry to		
Erythronic acid	136.10				discriminate		
Ribose	150.13				endogenous and		
Benzylazanium/o-toluidine/N-methyl-aniline	107.16				exogenous compounds		
N-Butylaniline/phentermine/2,6-diethylaniline	149.23				in exhaled breath		
3 Hexylpyridine	93.13				in exhared breading		
But-2-enoic acid	86.09	Headspace of	QToF	HRMS and isotopic	Fingerprinting Breast	10.1038/sr	
trans-2-Octenoic acid	142.20	cell culture	QIUI	patterns			
				patterns	Cancer vs. Normal	ep05196	
4-Hydroxynonenal	156.23 224.30	plates			Mammary Cells by Mass		
Methyl jasmonate					Spectrometric Analysis		
3-oxo-2-pentyl-cyclopentanebutanoic acid	240.34				of Volatiles		
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-heptadier							
3-Methyl-alpha-ionyl acetate	250.38						
diethyl ethylphosphonate (DEEP)	166.16	evaporated	Ion Trap	molecule known	Direct Quantification of	10.1021/a	
Diisopropyl methylphosphonate (DIMP)	180.18	from liquid		before injection	Chemical Warfare	c5035874	
malathion	330.36	sample			Agents and Related		
dichlorvos (DCV)	220.97				Compounds at Low ppt		
phoxim (PHX)	298.30				Levels: Comparing Active		
thiodiglycol (TDG)	122.19				Capillary Dielectric		
2-nonenal	140.22	breath	HRMS	HRMS followed by	Identification of 2-	10.1021/a	201
2-decenal	154.25		Orbitrap	HRMS-MS and	Alkenals, 4-Hydroxy-2-	c504796p	
2-undecenal	168.28			LCMSMS	alkenals, and 4-Hydroxy-		
2-dodecenal	182.3				2,6-alkadienals in		
2-tridecenal	196.33				Exhaled Breath		
2-tetradecenal	210.36				Condensate by UHPLC-		
4-hydroxy-2-hexenal	114.14				HRMS and in Breath by		
4-hydroxy-2-heptenal	128.17				Real-Time HRMS		
4-hydroxy-2-octenal	142.20				Redistine liking		
4-hydroxy-2-decenal	142.20						
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-terdecadienal	210.32						
4-hydroxy-2,6-tetradecadienal	224.34						
4-hydroxy-2,6-pentadecadienal	238.37						
Ketamine	237.73	in-vivo	QToF	MS/MS	Drug Pharmacokinetics	10.1002/a	
Norketamine	223.70	headspace of			Determined by Real-	nie.20150	
hydroxyketamine	253.73	mouse cage			Time Analysis of Mouse		
hydroxynorketamine	239.70	-			Breath		
dehydronorketamine	221.68						
propofol	178.27						
Valproic acid	144.21						
: methylfuran	82.10	Breath	HRMS	HRMS followed by	Real-Time High-	10.1021/a	
ethylfuran	96.13	Li Costi		HRMS-MS and	Resolution Tandem	cs.analch	
propylfuran	110.16		e.anap	LCMSMS	Mass Spectrometry	em.5b015	
butylfuran	124.18				Identifies Furan	09	
pentylfuran	138.21				Derivatives in Exhaled		
hexylfuran	196.24				Breath		
heptylfuran	166.26						
octylfuran	180.29						
nonylfuran	194.31						
decylfuran	208.34						
undcylfuran	222.37						
dodecylfuran	236.39						
formylfuran	97.09						
acetylfuran	110.12						
acetonefuran	126.15						
hydroxymethyl furan	98.10						
benzothiazole	135.19	Breath	QToF	HRMS followed by	Detection and	10.1021/a	
2-aminobenzothiazole	150.20	Sicult	4,01	HRMS-MS and LC-	Quantification of	cs.est.5b0	
2-aminobenzothiazole 2-mercaptobenzothiazole	150.20			MS/MS	Benzothiazoles in	3809	
2-hydroxybenzothiazole	151.19			way wa	Exhaled Breath and	3003	
	151.19						
2-methylthiobenzothiazole 2-(4-35 morpholinyl)benzothiazole	220.07				Exhaled Breath		
hexamethylene triperoxide diamine	220.07	evaporated	QToF	molecule known	Condensate by Real- Vapor Pressure of	10.1021/a	
	200.1/	from liquid sample	QIUF	before injection	Hexamethylene Triperoxide Diamine (HMTD) Estimated Using Secondary Electrospray Ionization Mass	10.1021/a cs.jpca.5b 08929	
Iconrono	69.10	D+1-	07-5	MAC /MAC	Spectrometry	10 1100 10	
Isoprene	68.12	Breath	QToF	MS/MS	The Effect of CPAP	10.1136/th	
2-pentenal	84.12				Withdrawal on Exhaled	oraxjnl-	
Methylphenol	324.40				Breath in Obstructive	2015-	
Homocysteine thiolactone	117.17				Sleep Apnea – A	207597	
Ethylphenol	122.16				Randomized Controlled		
Mevalonic acid	148.16				Trial		
Digitalose	178.18						

Identified species. Page 3 of 6

molecule	molar mass	sample type	detector	identification method	publication tittle	DOI	year
Melatonin	232.28	evaporated	HRMS	molecule known	Numerical Modeling and		2016
Acetaminophen	151.16	from liquid		before injection	Experimental Validation		2010
Pentobarbital	226.27	sample	Sienap	cerore injection	of a Universal Secondary		
Midazolam	325.78				Electrospray Ionization		
β-caryophyllene	204.36	in-vivo air in	HRMS	HRMS (MS & MS/MS)	Capturing in Vivo Plant	10.1021/a	-
3-hexenyl acetate	142.20	plant cage	Orbitrap		Metabolism by Real-	cs.analch	
monoterpene	136.23				Time Analysis of Low to	em.5b044	
sesquiterpene	204.36				High Molecular Weight	52	
hexenol	100.16				Volatiles		
methyl salicilate	152.15						
monoterpene alcohol	152.23						
hexenyl butyrate	170.25 150.26						
4,8-dimethylnona-1,3,7-triene (DMNT) 4,8,12-trimethyltrideca-1,3,7,11-tetraene (TMTT)	218.38						
monothiophene	98.17						
myosmine	146.19	dyrect	HRMS	HRMS (MS & MS/MS)	Real-Time Chemical	10.1002/c	
Acetyl Pyrazine	122.12	ecigarrete puff			Analysis of E-Cigarette	hem.2015	
Ethylmaltol	140.14				Aerosols By Means Of	04450	
Isoamyl isovalerate	172.26				Secondary Electrospray		
4-hydroxy-2-pentenal	100.11	Breath	HRMS	HRMS (MS & MS/MS)	Expanding metabolite	10.1088/1	
4-hydroxy-2,6-pentadienal	98.10		Orbitrap		coverage of real-time	752-	
4-hydroxy-2,6-hexadienal	112.13				breath analysis by	7155/10/1	
hexenoic acid	114.14				coupling a universal	/016010	
heptenoic acid	128.17				secondary electrospray		
nonenoic acid	156.22				ionization source and		
decenoic acid	170.25				high resolution mass		
undecylenic acid tridecylenic acid	184.27 212.32				spectrometry - A pilot study on tobacco		
pentadecylenic acid	240.38				smokers		
oxopentanoic acid	116.12				Shlokers		
oxoheptanoic acid	144.17						
oxononanoic acid	172.22						
oxooctenoic acid	186.25						
oxononenoic acid	200.28						
oxodecenoic acid	214.30						
heptenedioic acid	184.10						
octenedioic acid	198.13						
nonenedioic acid	212.16						
decenedioic acid	226.18	Descale	LIDIAC		Constant of the state of the st	10 1000/0	
Anthranilate 4,8-Dihydroxyquinoline	137.14 161.16	Breath	HRMS	HRMS (MS & MS/MS followed by HPLC-	Secondary electrospray ionization coupled to	10.1039/C 6CC03070J	
4,6-Dihydroxyquinoline	161.16		Orbitrap	MS-MS)	high-resolution mass	00000703	
3-Methyldioxyindole	163.17				spectrometry reveals		
Indole-3-acetate	175.18				tryptophan pathway metabolites in exhaled		
5-Hydroxyindoleacetaldehyde	175.18						
3-Hydroxykynurenamine	180.20				human breath		
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 6-Hydroxymelatonin	236.22 248.28						
Formyl-N-acetyl-5-methoxykynurenamine	246.26						
Ornithine	132.16	Breath	HRMS	HRMS (MS & MS/MS	Real-Time	10.1373/cl	1
Glycine	75.07			followed by HPLC-	Quantification of Amino	inchem.20	
Valine	117.15		· ·	MS-MS)	Acids in the Exhalome by		
Iso-leucine	131.17				Secondary Electrospray		
Phenylalanine	165.19				Ionization-Mass		
Lysine	146.19				Spectrometry: A Proof-of-		-
sulfate/sulfuric acid	98.08	Breath	HRMS	HRMS and isotopic	Direct human breath	10.1002/rc	
silicate/silicic acid	96.11		Orbitrap	patterns	analysis by secondary	m.7794	
nitrate/nitric acid	63.01				nano-ESI ultra-high		
dichlorobenzene	147.01				resolution mass		
polysiloxane (n=6)/Dodecamethylcyclohexasiloxane sulfosuccinate/sulfosuccinic acid					spectrometry:		
	198.15				Importance of high mass		
monoacylglycerol	330.50				resolution and mass		

	molar						
molecule	mass	sample type	detector	identification method	publication tittle	DOI	yea
acetic acid	60.05	Headspace of	HRMS	HRMS, isotopic	Rapid fingerprinting of	10.1016/j.f	201
β-ionone	192.30	fresh fruits	Orbitrap	patterns	grape volatile	oodcont.2	
(E,E)-2,4-heptadienal	110.15				composition using	017.04.041	
4-vinylphenol	120.15				secondary electrospray		
2,4-dinitrotoluene (DNT)	182.13	Air surrounding canine training	QQQ	molecule known	Direct Quantification of	10.1021/a	
2,6-dinitrotoluene (DNT)	182.13		(MS)	before injection	Chemical Warfare	cs.analch	
triacetone triperoxide (TATP)	222.24	samples			Agents and Related	em.7b004	
cyclohexanone	98.15				Compounds at Low ppt	51	
phthalatic anhydride	148.10	lab ambient air		HRMS HRMS, MS/MS & rbitrap isotopic patterns	Secondary electrospray	10.1039/C	
Dibutylphtalate	278.34				ionization proceeds: Via	7AY01121K	1
2,2,2-trifluoroethanol	100.04				gas-phase chemical		
ω-hydroxynonanoic acid	174.24	Breath	QToF	HRMS (MS & MS/MS followed by HPLC-	Mass-Spectrometric	10.1021/a	
ω-hydroxydecanoic acid	188.26				Detection of Omega-	cs.analch	
ω-hydroxyundecynoic acid	202.29			MS-MS)	Oxidation Products of	em.7b020	
ω-hydroxydodecynoic acid	216.32				Aliphatic Fatty Acids in	92	
ω-hydroxytridecynoic acid	230.34				Exhaled Breath		
ω-hydroxytetradecynoic acid	244.37						
ω-hydroxypentadecynoic acid	258.40						
ω-oxodecanoic acid	186.25						
ω-oxotridecynoic acid	228.33						

Identified species. Page 4 of 6

molecule	mass	sample type	detector	identification method	publication t	ittle
ω-oxotetradecynoic acid	242.35					
ω-oxopentadecynoic acid	256.38					
pentanedioic acid	132.11					
hexanedioic acid	146.14					
heptanedioic acid	160.17					
octanedioic acid nonanedioic acid	174.19					
nonanedioic acid decanedioic acid	188.22					
undecanedioic acid	202.25					
docecanedioic acid	230.30					
tridecanedioic acid	244.33					
tetradecanedioic acid	258.35					
pentadecanedioic acid	272.38					
salbutamol-4-0-sulfate	319.38	Breath	QToF	HRMS (MS & MS/MS	Metabolic e	effects
formoterol	344.41			followed by HPLC-	inhaled sal	lbutar
Methyl cinnamate	162.19	headspace of	HRMS	HRMS, Isotopic	Comprehen	sive R
Benzofuran	118.10	in-vivo yeast		labeled molecular	Time Analy	
1-Methylpyrrolo[1,2-a]pyrazine		culture fed with		formula compared	Yeast Volat	ilome
Vanillic acid	168.14	isotopically		with metabolomic		
Coixinden A	190.19	labeled		database		
Diatretin 2	145.11	glucose				
Indoleacrylic acid 4-Amino-2-methyl-1-naphthol	187.19 173.21					
PHENYL 2-PYRIDYL KETONE	1/5.21	Tł		mpounds are	all licto	d in
Ricinine	164.16					
Vanillin	152.15		the sa	me publicatio	n of 201	.7
4-hydroxy-3-nitrophenylacetate	197.14					
Oroselone	226.23	Distantes	arness!			224 3
Resveratrol	228.25	Dihydrof		6-octadiene		224.3
(3-Methyl-2-butenyl)-benzene	146.23		imetnyi-1, lisoborneo			138.2
3-Propylidene-1(3H)-isobenzofuranone	174.20		thyl-naph			156.2
3-(indol-3-yl)pyruvic acid	203.19			vclopentene		192.3
Dracunculin	220.18		ethylstyre			118.1
2-Heptanone	114.18		xyphenol			76.1
Cyclohexane	84.16		etradecan	oate		242.4
alpha-Amylcinnamyl isovalerate	288.42			ene-1-(1methylethyli	dene)-cycloh	150.2
Nerol	154.25	(Z)-1,5-TI	idecadier	ie		180.3
Ethyl vanillin	166.17	Propyl he	exanoate			158.2
Alpha-Ketoisovaleric acid 2-Undecanone	116.12 170.29	trans,tra	ns-2,4-deo	adienal		152.3
xi-1-Butoxy-1-methoxyethane	170.29		-4-octano	lide		156.2
isobutanol	74.12	beta-Cal				200.3
Ethyl decanoate	200.32	1,3-Buta				54.0
Cyclopentane	70.10		hyletheny	l)-3-(1-methylethyl)-b	enzene	160.2
Hexanediol	118.17	Serratol				290.4
4-Hydroxymethylpyrazole	98.10	Cembrer				272.4
Pyrrolidine	71.12	Geranic				168.2
(Z)-9-Cycloheptadecen-1-one	250.42	2,5-Dimethyl-4-ethoxy-3(2H)-furanone				150.2
Stearidonic acid	276.41	Carvone				130.1
Isopentyl hexanoate	186.29	Furaneo				128.1
Ethyl octanoate	172.26	Pyridoxa				167.1
Propyl decanoate	214.34		ydopamin	e		169.1
Octanedioic acid / dihexyl ester	342.51	Ambroni				236.3
Octadecanedioic acid	314.46	Zingeror	ne			194.2
Octanoic acid	144.21 282.46	Lavande	r lactone			126.1
Ethyl 9-hexadecenoate 1-Phenylheptane	282.46	Isomyris	ticin			192.2
alpha-Curcumene	202.33	Glycerol				92.0
Butylated hydroxytoluene	220.35		kadecanoa			284.4
1-octen-3-one	126.20			ctadien-3,7-dio		170.2
2-Isopropyl-1,4-hexadiene	124.22		uccinate			128.1
1.3-Octadiene	110.20	2-nonan				142.2
3-Methylcyclopentene	82.14		lcyclohexa			112.1
Benzene	78.11		-p-cymene			132.2
Toluene	92.14		ecenoate			198.3
1,3-Diisopropylbenzene	162.27	Sorbic ad		pyloxazole		112.1
1-Methyl-1,3-cyclohexadiene	94.15		anyl aceto			208.3
(Z)-1,3-Octadiene	108.18		anyi aceto thyl acetat			208.:
Ethylbenzene	106.16	Hexa-2,4		-		98.1
beta-Farnesene	204.35	Dendrol				218.3
1-Methyl-4-(1-methylpropyl)-benzene	148.24	Isogerm				216.3
Cumene	120.19			-2-butanol		164.2
Nerolidol	222.37			nyl-2-propenyl)-benze	ne	174.2
Santene P-Cymene	122.21	Dihydroa	actinidioli			180.2
P-Cymene Acetamide	134.22	Dihydroe	-			166.3
Acetamide Cyclopentadiene	59.07	1,4-Ipom				170.2
Quinaldic acid	173.17	Cyperotu				216.3
1-nitrosonaphthalene	157.17			1,3-propanediol		105.1
Myrcene	136.23		-1-propan			104.1
Vinyl caffeate	206.19		ydroxybut			132.1
4-Methylacetophenone	134.17		ydroxy pro	panoate		118.1
Syringol	154.16		anedione			100.1
Tyrosol	138.16	(R)-Aceto Norfurar				88.1
2-Furanmethanol	98.10	Norfurar				114.1 76.0
2-Acetolactate	132.11	propyler Propana				76.0 58.0
Trihydroxybutane	106.12	Capsidio				236.3
3-Dehydroxycarnitine	145.20			opyl-benzene		190.3
2,4-Dimethyl-2-pentene	98.19		but-2-ena			190.3
Geranyl valerate	238.36			ethylphenol		234.3
Continuos				enoic acid		252.3
Continues		2-Methyl				86.1
						94.1
		Phenol				94.1

Continues

Super SESI (Application Note) Identified species. Page 5 of 6

DOI

10.1088/1 10.1088/1 752-10.1038/s 41598-017-14554-y

year 2017

These compounds are all listed in the same publication of 2017

Ethyl 2-hexenoate	142.20
3-Oxooctanoic 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
Paullinic acid	310.51
Linoleic acid	280.44
1-Octen-3-ol	128.21
4-Vinylguaiacol	150.17
Succinic anhydride	100.07
Cycloserine	102.09
4-Hydroperoxy-2-nonenal	172.22
Geranyl acetone	194.31
Homodihydrojasmone	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-Tetrahydroridentin B	268.35
(±)-(Z)-2-(5-Tetradecenyl)cyclobutanone	264.44
Sinapyl alcohol	210.23
4-Pyridoxic acid	183.16
alpha-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-Octanovicarnitine	270.30
Dihydrogeranylacetone	196.33
gamma-Undecalactone	196.55
Citronellyl propionate	212.33
8-Heptadecenal	252.43
Citral	152.24
Butanoic acid	88.11
	88.11
ethylexanoate	
diacetyl	86.09
2-phenyl ethanol	122.16
nona-2,6-dienal	138.21

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Alpha Choirage Delutere National source Senands	Malate /malic acid	134.09	Breath	HRMS	HRMS (MS & MS/MS			-
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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.

Super SESI (Application Note)

Identified species. Page 6 of 6