



Research article

Organic compounds associated with microplastic pollutants in New Jersey, U.S.A. surface waters

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Table 1. Tentatively Identified Compounds (TICS) > 1 ng in 28 samples.

#	CAS Number	Compound names of tentatively identified compounds (TICS)	Amount (ng) in 28 samples	Description	Uses/Reference
1	5650-44-2	Methcathinone	679.63	Monoamine alkaloid and psychoactive stimulant, a substituted cathinone. Used as a recreational drug due to its potent stimulant and euphoric effects and is considered to be addictive, with both physical and psychological withdrawal occurring if its use is discontinued after prolonged or high-dosage administration. No clinical use.	Pharmaceutical International Narcotics Control Board – Green List. 2017, Schedule I Controlled Substance
2	83-34-1	Indole, 3-methyl-	509.58	3-methylindole; a mildly toxic white crystalline organic compound in the indole family. Occurs naturally in feces and coal tar; found in several flowers and essential oils. Used as a fragrance and fixative in many perfumes and as an aroma compound.	Natural Compound Fragrance Use Pub Chem Open Chemistry Database The Good Scents Co.
3	1349245-31-3	Naphyrone 1-naphthyl isomer	421.66	Designer drug producing stimulant effects	Research Applications Bertin Bioreagent
4	3658-80-8	Dimethyl trisulfide	421.64	Product of bacterial decomposition; produced by various plant species	Natural Compound Pub Chem Open Chemistry Database
5	None	5-Thiazolecarboxamide, N-(4-chloro-2,5-d	420.60	Antitumor, antibacterial; kinase inhibitor	Pharmaceutical www.mdpi.com
6	65996-50-1	Pyrolo[3.2-d]pyrimidin-2,4(1H,3H)-dione	266.95	Used for the preparation of pyrazolopyrimidine derivatives or analogs thereof as CCR4 function modulators	Laboratory Chemical Pub Chem Open Chemistry Database
7	112-84-5	13-Docosenamamide, (Z)-	178.57	Cerebrospinal fluid of rats and humans. Causes reduced mobility and slightly lessened awareness. Erucylamide	Natural Compound Food Additive, Anti-Adhesive, Lubricant, Food packaging, Building construction materials Pub Chem Open Chemistry Database
8	54060-30-9m-	Aminophenylacetylene	94.45	Used in the synthesis of benzoxazine monomers	Laboratory Chemical
9	14901-07-63-	Buten-2-one, 4-(2,6,6-trimethyl-1-cycl	60.67	Used in perfumery	Flavor & Fragrance Agent Good Scents Co.
10	None	1-naphthalenesulfonamide, 5-(acetyloxy)-	60.62	Food additive	
11	5756-24-1	Tetrasulfide, dimethyl	60.47	Flavoring substance authorized for use in foodstuffs	Flavoring Use Good Scents Co.
12	5989-27-5	D-Limonene	45.46	Major component in oil of citrus fruit peels. The D-isomer occurs more commonly in nature as the fragrance of oranges. A flavoring agent in food manufacturing	Natural Substance Flavoring Use Pub Med.gov - NCBI
13	5655-61-8	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimeth	42.83	Perfuming agent	Fragrance Use God Scents Co.

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
14	7239-23-8	3-Dodecene, (Z)-	39.84	Natural substances and extractives. Synthesis, properties, and applications of heterocyclic organic compounds important in most pharmaceuticals, biomass (cellulose and related materials), and many natural and synthetic dyes.	Laboratory Chemical Pub Chem Open Chemistry Database Good Scents Co.
15	77143-15-8	Furan, 2-methyl-5-(1,1,5-trimethyl-5-hexenyl)-	38.83		Research Chemical Pub Chem Open Chemistry Database www.chemeo.com
16	None	1-Benzoxirene, 5a-[3-oxo-1-butenyl]perhy	37.95		
17	49686-56-8	Cephalotaxine, 11-(acetyloxy)-, acetate	32.03		
18	67-96-9	Dihydrotachysterol	30.43	A synthetic vitamin D analog	Pharmaceutical Pub Chem Open Chemistry Database
19	88395-46-4	Isospathulenol	24.88	Human body, found in cell membrane and cytoplasm, alcoholic beverages, herbs, species, tea	Natural Compound Pub Chem Open Chemistry Database Good Scents Co.
20	20307-84-0	Cyclohexene, 4-ethenyl-4-methyl-3-(1-met	24.61	Food additive delta Elemene	Human Metabolome Database Flavor Agent Pub Chem Open Chemistry Database Good Scents Co.
21	88-29-9	7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetra	22.57	Used in perfumes (musk) Versalide	Fragrance Use Pub Chem Open Chemistry Database Good Scents Co.
22	None	Z,Z-3,15-Octadecadien-1-ol acetate	21.77		Pub Chem Open Chemistry Database
23	24703-35-3	(1S,2E,6E,10R)-3,7,11,11-Tetramethylbicy	21.65	Bicyclogermacrene - green woody floral Food additive	Natural Compound Favoring Agent Pub Chem Open Chemistry Database Good Scents Co.
24	None	Cobalt, bis(1,3-diisopropyl cyclopentadiene	20.92		
25	117-81-7	Bis(2-ethylhexyl) phthalate (plasticizers, PVC indicator)	20.39	Bis(2-ethylhexyl) phthalate (DEHP) the most common member of the class of phthalates which are used as plasticizers Indirect food additive	Plasticizer Adhesives & Coatings Pub Chem Open Chemistry Database Good Scents Co.
26	345991-15-N-3	(3,5-Bis-trifluoromethyl-phenyl)-2-met	20.01		
27	17283-81-72	Butanone, 4-(2,6,6-trimethyl-1-cyclohe	19.15	Dihydro-beta-ionone – woody Perfuming agent Toxic to aquatic life	Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database Laboratory Chemical Safety Summary
28	56687-67-3	Cyclopropaneoctanoic acid, 2-[(2-pentylc	18.37	DCPLA methyl ester -	Research www.ChemSrc.com
29	80625-30-5	1,E-8,Z-10-Tridecatriene	17.76		Research www.Guidechem.com
30	1502-05-2	Cyclodecanol	16.70	Cyclodecyl alcohol	Laboratory Chemical Pub Chem Open Chemistry Database Good Scents Co.

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
31	None	Z,Z-3,15-Octadecadien-1-ol acetate	15.88	NIST #130954	Research Pub Chem Open Chemistry Database
32	3796-70-1	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)	15.50	(E)-geranyl - floral, green fruity	Flavor & Fragrance Use Good Scents Co.
33	629-98-1	13-Docosen-1-ol, (Z)-	15.49	Erucyl alcohol; long chain fatty alcohol	Pharmaceutical/Chemical Synthesis Good Scents Co. Pub Chem Open Chemistry Database
34	22725-64-0	Octacosanal	15.16	Isolated from wax of wine grapes and cabbage leaves; found in alcoholic beverages	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
35	544-63-8	Tetradecanoic acid	13.40	Myristic Acid; waxy food additive	Natural Compound Cosmetic & Food Additive Good Scents Co. Pub Chem Open Chemistry Database
36	464-49-3	(+)-2-Bornanone	13.19	Dextro-camphor - methol, minty	Flavor & Fragrance Agent Good Scents Co. NIST Chemistry Web Book
37	127-41-3	.alpha.-Ionone	13.14	Sweet, woody, floral, fruity; widely used in perfume composition; synthetic flavoring substance permitted for human consumption	Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
38	695-12-5	Cyclohexane, ethenyl-	12.93	Vinylcyclohexane; highly flammable, fatal in swallowed; very toxic to aquatic life	Laboratory Chemical Pub Chem Open Chemistry Database
39	62199-51-3	Cyclopentane, 1-pentyl-2-propyl-	12.75	NIST #61268	Research Pub Chem Open Chemistry Database
40	4707-47-5	Benzoic acid, 2,4-dihydroxy-3,6-dimethyl	12.08	Veramoss; mossy, woody synthetic compound; irritating to eyes, skin	Flavor & Fragrance Agent Good Scent Co. Pub Chem Open Chemistry Database
41	83489-22-9	1,E-4,Z-8-Dodecatriene	11.75		Research www.ChemSrc.com
42	25152-84-5	2,4-Decadienal, (E,E)-	11.70	Fatty, fried flavoring agent	Flavor Agent Good Scents Co. Pub Chem Open Chemistry Database
43	719-22-2	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,	11.67		Laboratory Chemical Pub Chem Open Chemistry Database
44	551-93-9	Ethanone, 1-(2-aminophenyl)-	11.55	2-aminoacetophenone	Flavor Agent Good Scents Co.
45	None	Z,Z,Z-4,6,9-Nonadecatriene	11.49		Pub Chem Open Chemistry Database
46	31499-72-6	2-Butanone, 4-(2,6,6-trimethyl-2-cyclohe	10.77	Dihydro-alpha-ionone - berry, floral	Natural Compound Flavor & Fragrance Use Good Scents Co. Pub Chem Open Chemistry Database
47	6217-54-5	Doconexent (fatty acid)	10.73	Essential fatty acid; most abundant ω -3 fatty acid in neural tissues, especially in the retina and brain. Supplementation of dietary DHA inhibits progression of atherosclerosis and delays photoreceptor degeneration in <i>retinitis pigmentosa</i>	Natural Compound Pharmaceutical Use Good Scents Co.

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
48	118-65-0	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trime	10.41	Isocaryophyllene - woody, spicy plant produced (allspice, anise, basil, chamomile, cinnamon, clove, lemon verbena, other Anti-inflammatory Agent	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
49	87-44-5	Caryophyllene	10.40	Beta-caryophyllene – spicy Additive – spice blends, chewing gum, soaps, detergents	Flavor & Fragrance Agent Good Scents Co.
50	483-76-1	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-	10.39	Delta-cadinene - herbal, woody Plant compound (allspice, anise, basil, bay leaf, other)	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
51	150320-52-8	Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-m	10.18		Research www.ChemSrc.com
52	6753-98-6	Humulene	10.17	Naturally occurring monocyclic sesquiterpene; Humulene has been found in many aromatic plants on all continents	Natural Compound Flavoring Agent Good Scents Co. Pub Chem Open Chemistry Database
53	2277-20-5	6-Nonenal, (E)-	10.16		Flavoring Agent Good Scents Co. Pub Chem Open Chemistry Database
54	85763-57-1	11-Methyldodecanol	10.15	Isotridecyl alcohol Biochemical for proteomics research	Laboratory Chemical Good Scents Co. Pub Chem Open Chemistry Database
55	17092-92-1	(4H)-Benzofuranone, 5,6,7,7a-tetrahydro	10.07	Safflower flower, black tea Musk coumarin	Natural Compound Flavoring Agent Good Scents Co. Pub Chem Open Chemistry Database
56	2734-47-6	5,8,11,14,17-Eicosapentaenoic acid, meth	10.04	Precursor for resolvins, mediators that help resolve inflammatory processes	Pharmaceutical Pub Chem Open Chemistry Database
57	5090-61-9	(2R,8R,8aS)-8,8a-Dimethyl-2-(prop-1-en-2	9.65	Citrus fruits – lemon, mandarin, orange Nootkatene -	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
58	7239-23-8	3-Dodecene, (Z)-	9.61	Acyclic olefin	Natural Compound Research Good Scents Co. Pub Chem Open Chemistry Database
59	1560-89-0	Heptadecane, 2-methyl-	9.58		Natural Compound Research Good Scents Co. Pub Chem Open Chemistry Database
60	36577-33-0	(1R,3aS,8aS)-7-Isopropyl-1,4-dimethyl-1,	9.48	Guaia-6,9-diene	Research Pub Chem Open Chemistry Database
61	6175-49-1	2-Dodecanone	9.46	Decyl methyl ketone, found in alcoholic beverages, blue cheese, cocoa, hop oil, milk Citrus, fatty	Natural Compound Flavoring Agent Good Scents Co. Pub Chem Open Chemistry Database
62	619-62-5	4-Isopropyl-1-methylcyclohex-2-enol	9.44	Para-2-menthen-1-ol; herbal	Natural Compound Research Good Scents Co. Pub Chem Open Chemistry Database
63	150-86-7	Phytol	9.28	Floral; emollient, masking and perfuming agent; constituent of chlorophyll; found in beef fat, cheddar cheese, cinnamon, kelp, lemon balm, black tea. Precursor for synthetic manufacture of vitamin E and vitamin K1.	Natural Compound Flavoring Agent Vitamin production Good Scents Co. Pub Chem Open Chemistry Database

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
64	None	4-Methyl-3,5-decandione	9.12		
65	1569-60-4	5-Hepten-2-ol, 6-methyl-	8.73	Coriander heptenol; sweet, oily; found in herbs and spices	Natural compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database Research
66	108511-85-9	2-Hydroxy-1,1,10-trimethyl-6,9-epidioxyd	8.68	NIST #212109	Pub Chem Open Chemistry Database Research
67	24828-58-8	Cyclopentene, 3-undecyl-	8.52		
68	None	1-Benzoxirene, 5a-[3-oxo-1-butenyl]perhy	8.51		
69	None	Oxalic acid, butyl 2-isopropyl phenyl ester	8.51		
70	55124-79-3	Heptadecane, 9-hexyl-	7.98	NIST #15194	Research Pub Chem Open Chemistry Database
71	78-70-6	Linalool	7.98	Widespread natural occurrence; Citrus, floral used very extensively in perfume compositions of almost all types; denaturant	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database Research
72	150320-52-8	Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-m	7.84		www.Guidechem.com
73	None	Z,E-3,13-Octadecadien-1-ol	7.79		
74	432-25-7	1-Cyclohexene-1-carboxaldehyde, 2,6,6-tr	7.72	Beta-cyclocitral; tropical, saffron; Perfuming agent	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database Cannabis Testing Reference Standard LGC Quality – ISO Guide 34
75	7/3/4630	Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-	7.66	Valencene	
76	10374-74-07	Tetradecene	7.64	Biochemical for proteomics research	Laboratory Chemical Santa Cruz Biotechnology
77	488-97-1	Tricyclo[2.2.1.0(2,6)]heptane, 1,3,3-tri	7.55	Cyclofenchene	Natural Compound Research Good Scents Co. Pub Chem Open Chemistry Database
78	489-77-0	6-Isopropyl-1,4-dimethylnaphthalene	7.39	Drug for dermatological disorders & disorders of the nervous system	Pharmaceutical Pub Chem Open Chemistry Database
79	6831-16-9	(-)-9-Aristolene	7.04	Aristolene	Natural Compound Laboratory Chemical Good Scents Co. Pub Chem Open Chemistry Database
80	75023-40-4	1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-me	7.02	Helminthogermacrene	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
81	5951-61-1	Naphthalene, 1,2,4a,5,8,8a-hexahydro-4,7	6.89	Cadinenes are bicyclic sesquiterpenes that occur in a wide variety of essential oil-producing plants; emitted from marijuana	Natural Compound Rice & Koziel. 2015. http://dx.doi.org/10.1016/j.dib.2015.09.053
82	693-54-9	2-Decanone	6.71	Methyl octyl ketone; floral peach odor, fermented cheesy taste; Plant metabolite found in corn, cheese, other	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database Research
83	None	14-Oxatricyclo[9...1.0(1,1 0)]tetradecan	6.65		MOL Instincts

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
84	10208-80-7	alpha.-Muuroleone	6.61	Found in allspice, anise, basil, clover, corn, other plants	Natural Compound Flavoring Agent Good Scents Co. Pub Chem Open Chemistry Database
85	118-56-9	Homosalate	6.54	Organic compound used in sunscreens as a chemical UV filter; identified as an antiandrogen in vitro. Has estrogenic activity toward estrogen receptors α , and general in vitro estrogenic activity. Evidence homosalate can break down into more toxic products	Cosmetic Additive Antioxidant, stabilizer Good Scents Co. Pub Chem Open Chemistry Database
86	None	Morphinan-4,5-epoxy-3,6-di-ol, 6-[7-nitr	6.43	NIST #129096	Pub Chem Open Chemistry Database
87	5452-99-3	2,5-Dimethoxy-2'-hydroxychalcone	6.39	Docos-13-ynoic Acid	Research Chemical www.letopharm.com
88	73209-42-4	trans-Calamenene	6.32	(E)-calamenene	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
89	None	Succinic acid, nonyl tetrahydrofurfuryl	6.28		Research MOL Instincts
90	None	13-Tetradecene-11-yn-1-ol	6.25	NIST #131004	Pub Chem Open Chemistry Database
91	33156-93-3	[(Z)-1-Butenyl]-1,4-cycloheptadiene	6.25	Ectocarpene - vitiver oil	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
92	483-77-2	Naphthalene, 1,2,3,4-tetrahydro-1,6-dime	6.06	Calamenene is a metabolite of <i>Turnera diffusa</i> native to Central & So. America, commercially cultivated in Mexico & Bolivia. Found in allspice, basil, bay leaf, dill, oregano, black pepper, other plants	Natural Compound Good Scents Co. Pub Chem Open Chemical Database
93	80060-76-0	(Z)-18-Octadec-9-enolide	6.00		Research www.chemeo.com
94	51760-35-1	9,11-Dodecadien-1-ol, acetate, (Z)-	5.86		
95	88-58-4	1,4-Benzenediol, 2,5-bis(1,1-dimethyleth	5.69	di-tert-butyl hydroquinone Selective inhibitor of endoplasmic reticulum Ca ²⁺ ATPase	Laboratory Chemical Pub Chem Open Chemistry Database Good Scents Co.
96	25144-04-1	Cyclopentanol, 2-methyl-, trans-	5.66	Trans-2-methylcyclopentanol	Pharmaceutical Laboratory Chemical Pub Chem Open Chemical Database
97	19780-12-25	Dodecyne	5.56	Biochemical for proteomics research; cosmetic additive	Laboratory Chemical ChemSynthesis Chemical database
98	41977-47-3	Bicyclo[4.1.0]heptane, 3-methyl-	5.52	3-methylbicyclo[4.1.0]heptane	Research Pub Chem Open Chemistry Database
99	None	Fumaric acid, ethyl 3-fluorophenyl ester	5.47		
100	72150-30-2	Prost-13-en-1-oic acid, 9-(methoxyimino)	5.47		
101	50286-30-1	E-9-Tetradecenoic acid	5.40	Myristelaidic acid (9E-tetradecenoic acid) is a fatty acid lipid molecule	Natural Compound Laboratory Chemical Pub Chem Open Chemistry Database
102	330207-53-9	E-14-Hexadecenal	5.34	Application for agricultural pheromone patent (2016)	Pub Chem Open Chemistry Database

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
103	42474-44-2	Disulfide, methyl (methylthio)methyl	5.34	2,3,5-trithiahexane; sulfurous onion; found in brassicas species, oil of hops, Camembert cheese	Natural Compound Flavoring Agent Good Scents Co. Pub Chem Open Chemistry Database
104	5/4/2728	Benzamide, N,N-diethyl-4-methyl-	5.29	N,N-Diethyl-P-2toluamide Patent to treat seborrheic keratosis (2003-10-09)	Pharmaceutical Pub Chem Open Chemistry Database
105	142878-08-8	(3S,3aS,8aR)-6,8a-Dimethyl-3-(prop-1-en-	5.13	Trans-dauca-8,11-diene	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
106	15780-36-6	Bicyclo[2.2.1]heptane-2-carboxaldehyde,	5.09		
107	None	1,3,14,16-Nonadecatetraene	5.08		Research MOL Instincts
108	20851-55-24	Hepten-1-ol	5.07	Patents Pending; Found in pepper, chili, malt whiskey	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
109	560-32-7	1H-3a,7-Methanoazulene, 2,3,6,7,8,8a-hex	5.05	Alpha-patchoulene Found in pineapple fruit, patchouli oil	Natural Compound Good Scents Co.
110	17540-75-9	Phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-	4.88	4-sec-butyl-2,6-di-tert-butyl phenol Industry Uses – functional fluids, lubricants, process regulators, processing aids	Laboratory Chemical Indirect Food Additive Adhesives and Coatings Good Scents Co. Chem Pub Open Chemical Database
111	2938-98-9	2-Methyl-1,4-butanediol	4.76		Industrial Chemical www.guidechem.com
112		8,10-Dodecadien-1-ol, (E,E)-	4.63	Codlure is an insecticide that controls fruit moth in apple and pear orchards Pesticide patents	Natural Compound Agrochemical Insecticide Good Scents Co. Pub Chem Open Chemistry Database
113	487-70-7	2,4,6-Trihydroxybenzaldehyde	4.51	Reactant involved in synthesis of 2,4,6-trichlorophenyl hydrazones with potential inhibition of protein glycation and Xanthine oxidase inhibitors. Generated by unspecified-gutmicro enzyme by human gut microbiota	Natural Compound Laboratory Chemical Pharmacology Patents Pub Chem Open Chemistry Database Good Scents Co.
114	None	Z-1,6-Tridecadiene	4.45	NIST #130983	Research Human Metabolome Database Pub Chem Open Chemistry Database
115	41977-46-2	Bicyclo[4.1.0]heptane, 2-methyl-	4.36		
116	None	5-Nonadecen-1-ol	4.22	Patent: Golf ball coating compositions (2007-07-24)	Pub Chem Open Chemistry Database
117	1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	4.04	Ketosisophorone; musty, wood, citrus; found in herbs and spices, tea, clover, honey, and saffron	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
118	None	3,19:14,15-Diepoxypregnan-20-one, 3,11,1	3.97		

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
119	506-32-1	Arachidonic acid (fatty acid)	3.94	Arachidonic acid is an essential unsaturated fatty acid present in cell membrane phospholipids; key inflammatory intermediate; can act as a vasodilator; emollient, skin conditioner	Natural Compound Food Additive Cosmetic Additive
120	18720-66-63	Heptanol, 6-methyl-	3.84	6-Methylheptan-3-ol	Natural Compound Laboratory Chemical Pub Chem Open Chemistry Database Good Scents Co.
121	13466-78-9	Delta 3-Carene	3.71	Citrus, terpenic odor; perfuming agent; found in turpentine, allspice, orange, basil, anise, cinnamon, citronella, others	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database Pub Chem Open Chemistry Database
122	None	Z,Z-3,15-Octadecadien-1-ol acetate	3.64		
123	472-66-2	1-Cyclohexene-1-acetaldehyde, 2,6,6-trim	3.56	Beta-homocyclocitral; camphoreous; perfuming and food additive agent	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database Pub Chem Open Chemistry Database
124	None	Z,Z,Z-4,6,9-Nonadecatriene	3.47		Pub Chem Open Chemistry Database
125	None	Z,E-2,13-Octadecadien-1-ol	3.41		Pub Chem Open Chemistry Database
126	None	Z-1,6-Tridecadiene	3.39		Pub Chem Open Chemistry Database
127	56318-84-45	Pentylcyclohexa-1,3-diene	3.22		
128	None	Morphinan-4,5-epoxy-3,6-di-ol, 6-[7-nitr	3.18		Pub Chem Open Chemistry Database
129	None	2-Pentadecanol acetate	3.18		
130	2219-84-3	Phenol, 2-methyl-4-(1,1,3,3-tetramethylb	3.14		Research www.Chemicalbook.com
131	765-05-9	Decane, 1-(ethenyloxy)-	3.11	Decyl vinyl ether; clean, rose perfuming agent;	Fragrance Agent Good Scents Co., Pub Chem Open Chemistry Database Pub Chem Open Chemistry Database
132	40467-04-72	Hexene, 2,5,5-trimethyl-	3.07		
133	119-84-6	3,4-Dihydrocoumarin	3.03	Benzodihydropyrone found in green vegetables; plant metabolite derived from coumarin; Coconut, vanilla, spicy, creamy	Natural Compound Flavoring Agent Good Scents Co. Pub Chem Open Chemistry Database
134	None	i-Propyl 7,10,13,16,19-docosapentaenoate	2.99		
135	112-23-2	Formic acid, heptyl formate	2.94	Food additive; perfuming agent; Green, waxy, floral	Flavoring & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database Research www.chemspider.com
136	22735-58-66	Butyl-1,4-cycloheptadiene	2.88		
137	132156-64-9	t-Butyl-4-iodo-2,2-dimethyladamantane	2.85		
138	None	Benzeneacetic acid, 6-ethyl-3-octyl ester	2.80		
139	2306-78-7	Nerolidyl acetate	2.78	Perfuming agent; fresh, sweet, citrus; found in herbs and spices, geranium, ginger, sage, other	Natural Compound Fragrance Use Good Scents Co. Pub Chem Open Chemistry Database

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
140	None	4,4-Dimethyladamantan-2-ol	2.72		
141	14912-44-8	Alpha-Ylangene	2.71	Found in bay leaf, cardamom, cinnamon, clove, corn, rosemary, thyme, others	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
142	5/8/2883	Octane, 2-cyclohexyl-	2.68		Research Pub Chem Open Chemistry Database
143	3886-78-0	cis-p-Mentha-2,8-dien-1-ol	2.66		Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
144	56554-35-99,	17-Octadecadienal, (Z)-	2.65		Industrial Chemical www.chemindustry.com
145	76920-33-7	1-Phenanthrenecarboxylic acid, 1,2,3,	2.64		
146	207974-19-4	2,3-Difluoromandelic acid	2.59		Industrial Chemical www.rdchemicals.com
147	90-26-6	Benzeneacetamide, .alpha.-ethyl-	2.58	Geristerol; 2-Phenylbutyramide	Biomedical Chemical Pub Chem Open Chemistry Database www.mpbio.com
148	1222-05-5	Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-	2.57	Galaxolide is a mixture of isomers; synthetic musk perfuming agent; EPA's assessment found it to be moderately persistent and bioaccumulative and highly toxic to aquatic organisms; sweet, floral	Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
149	72437-56-0	Disulfide, isopentyl methyl	2.57	Sulferous roasted	Natural Compound Flavoring Agent Good Scents Co. Pub Chem Open Chemistry Database
150	72437-68-4	Methyl pentyl disulfide	2.54	Sulferous onion; found in chives	Natural Compound Flavoring Agent Good Scents Co. Pub Chem Open Chemistry Database
151	None	5-Hydroxy-5-isopropyl-6-methyl-hepta-3,6	2.52		
152	123123-38-6	7-epi-a-Eudesmol	2.44		Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
153	55255-86-21-	Hexadecanone, 1-cyclopentyl-	2.42		Research www.Guidechem.com
154	None	Perhydroindene-4-carboxylic acid, 6-acet	2.41		
155	83406-41-1	1,8(2H,5H)-Naphthalenedione, hexahydro-8	2.41		Industrial Chemical www.lookchem.com
156	None	Pentadec-7-ene, 7-bromomethyl-	2.40		Pub Chem Open Chemistry Database
157	766-92-7	Benzyl methyl sulfide	2.39	Roasted burnt; present in cooked meat	Flavoring Agent Good Scents Co. Pub Chem Open Chemistry Database
158	3282-53-9	Cyclohexene, 1-butyl-	2.38	Present in heated beef fat; Intermediate in various industrial processes	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
159	82462-31-5	Eudesma-2,4,11-triene	2.34		Natural Compound Good Scent Co. Pub Chem Open Chemistry Database
160	None	tetramethyl 2,2',2",2'''- (cyclohexane-1	2.30		
161	None	Isonicotinic acid, 2-phenylethyl ester	2.29		
162	60-33-3	9,12-Octadecadienoic acid (Z,Z)-	2.27	Linoleic acid; Cosmetic Additive - antistatic, emollient, surfactant, hair and skin conditioning, cleansing agent; essential mammalian fatty acid occurring widely in plant oils	Natural Compound Cosmetic Additive Good Scents Co. Pub Chem Open Chemistry Database
163	2408-37-9	Cyclohexanone, 2,2,6-trimethyl-	2.21	Pungent citrus odor; present in bilberries, passion fruit, apricot, oats, carob, tea and other.	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
164	None	4b,8-Dimethyl-2-isopropylphenanthrene, 4	2.20		
165	80-26-2	.alpha.-Terpinyl acetate	2.19	Perfuming and flavoring agent; herbal, spicy, citrus; found in cardamom, grapefruit, eucalyptus, lemon, lime, others	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
166	88725-82-02,4,4-	Trimethyl-3-(3-methylbutyl)cyclohexyl	2.11		Research www.Guidedchem.com
167	None	Acetic acid, phenyl-, 3-hexenyl ester	2.10		
168	55955-46-93-	Buten-2-one, 4-(2-hydroxy-2,6,6-trimethyl-3-butyl)-	2.07		
169	460-16-2	Ethene, 1-chloro-2-fluoro-	2.06		Research Pub Chem Open Chemistry Database www.chemicalbook.com
170	36431-60-45-	Ethylcyclopent-1-carboxaldehyde	2.04	Compound identified in tomato	Natural Compound Pub Chem Open Chemistry Database Buttery & Takeoka (2004)
171	7795-95-1	1-Octanesulfonyl chloride	2.03		Laboratory Chemical Santa Cruz Biotechnology
172	None	Carbonic acid, eicosyl vinyl ester	2.02		
173	70000-19-0	Bicyclo[9.3.1]pentadecane-3,7-dien-12-ol,	1.97	Natural verticillol	Natural Compound Research Pub Chem Open Chemistry Database www.ChemSrc.com
174	78210-68-12-	Oxo-1-methyl-3-isopropylpyrazine	1.94		
175	106-24-1	Geraniol	1.93	Floral; personal care, household, soaps, detergents, perfumes; Standardized chemical allergen found in almonds, palmarosa oil, and geranium oil	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
176	None	1,3-Cyclohexanedione, 4,6-di-t-butyl-	1.92		
177	473-08-5	7-Isopropenyl-1,4a-dimethyl-4,4a,5,6,7,8	1.90	Alpha-cyperone	Natural Compound Research Good Scents Co. Pub Chem open Chemistry Database

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
178	36258-08-9	trans-(2-Ethylcyclopentyl)methanol	1.86		Research www.chemeo.com
179	150-86-7	Phytol	1.85	Floral; balsamic; emollient, masking and perfuming agent; used in making synthetic forms of Vitamin E and Vitamin K1; decomposition product of chlorophyll; found in beef fat, cheddar cheese, cinnamon, kelp, lamb liver, lemon balm, tea, witch hazel, others	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
180	89-83-8	Thymol	1.77	Phenolic, spicy; denaturant, hair dyeing, masking agent; pharmaceutical preparation stabilizer; antiseptic, antibacterial, and antifungal; cigarette additive	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
181	43219-80-3	(1R,4S,5S)-1,8-Dimethyl-4-(prop-1-en-2-yl)	1.76		Biochemical www.Pherobase.com
182	206-44-0	Fluoranthene	1.72	Polycyclic aromatic hydrocarbon found in many combustion products. Presence is an indicator of less efficient or lower-temperature combustion	Industrial Santa Cruz Biotechnology
183	97231-35-1	Cyclopropanecarboxaldehyde, 2-methyl-2-(1.71	Citrus	Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
184	871660-96-7	Panaginsene	1.68	Found in ginseng	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
185	18650-13-02	15-Hexadecanedione	1.67	Industrial chemical	www.chemicalbook.com
186	None	Methyl 5,13-docosadienoate	1.66		
187	58757-86-1	6-(2-propynyloxy)-1-hexanol	1.66		Research www.chemSrc.com
188	88-84-6	.beta.-Guaiene	1.65	Woody; cosmetic, perfume agent	Natural Compound Flavor & Fragrance Use
189	None	3-[2-(Adamantan-1-yl-oxo)-ethyl]-5-ethyl-	1.65		
190	135118-51-3	((4aS,8S,8aR)-8-Isopropyl-5-methyl-3,4,4	1.65	Hydroxy-alpha-murolene	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
191	88395-46-4	Isospathulenol	1.64	Primarily located in the cell membrane (predicted from logP) and cytoplasm. Found in alcoholic beverages, herbs and spices and tea.	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
192	14803-30-6	Cyclopropane, trimethyl(2-methyl-1-prope	1.57		Research www.guidechem.com
193	3777-70-6	Furan, 2-hexyl-	1.54	Found in roast chicken, roast lamb fat, roast peanut oil, cooked port, coriander oil, chickpea seed, others	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
194	6627-74-3	2-Cyclohexene-1-methanol, 2,6,6-trimethy	1.53	alpha-Cyclogeraniol	Research www.chemSrc.com

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
195	1126-65-4	Cyclopentane, 1,1'-thiobis-	1.52	Dicyclopentyl carbonate	Research www.chemicalbook.com
196	17671-27-1	Docosanoic acid, docosyl ester	1.48	Behenyl behenate; emollients, skin conditioning, perfuming agent	Cosmetic Additive Good Scents Co. Pub Chem Open Chemistry Database
197	None	2-Methyl-Z-7,8-epoxyhexadecane	1.41		
198	6728-26-3	2-Hexenal, (E)-	1.40	Green, leafy; Found in fruits, vegetables, spices; antibacterial agent and a plant metabolite	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
199	700-13-0	1,4-Benzenediol, 2,3,5-trimethyl-	1.39	Trimethylhydroquinone is a product for proteomics research	Laboratory Chemical www.chemicalbook.com
200	None	4-Methyl-4-nonadecene	1.37		
201	2416-20-8	Hexadecenoic acid, Z-11-	1.36	Intermediate in silkworm pheromone biosynthesis	Natural Compound Good Scents Co. Pub Chem Open Chemistry Database
202	7133-36-0	Cyclopentane, (methylthio)-	1.36	Pharmaceutical patents	Pub Chem Open Chemistry Database
203	87984-82-5	13S-Hydroxy-9Z,11E,15Z-octadecatrienoic	1.33		Research Santa Cruz Biotechnology
204	6971-40-0	17-Pentatriacontene	1.32		Research Pub Chem Open Chemistry Database
205	52474-77-8	Lanostan-12-one	1.31		Researchj www.chemicalbook.com
206	489-28-1	.alpha.-Maaliene	1.28		Natural Compound Good Scents Co. Research www.chemeo.com
207	267665-20-3	(1S,4S,4aS)-1-Isopropyl-4,7-dimethyl-1,2	1.27		Research www.chemeo.com
208	None	7-Oxabicyclo[3.3.1]non-2-ene, 8-(4-methoxydodecanoyl)-	1.25		
209	None	Phenol, 2-[3-oxododecanoyl]-	1.25		
210	107-90-4	Butanimidamide	1.23	Butyramidine	Research www.lookchem.com
211	104-93-8	Benzene, 1-methoxy-4-methyl-	1.22	Para-methyl anisole; perfuming agent; found in tomato, ylang-ylang, Camembert cheese, lavender	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
212	None	Butylphosphonic acid, 2-cyclohexylethyl	1.22		
213	472-66-2	1-Cyclohexene-1-acetaldehyde, 2,6,6-trim	1.22	Beta-homocyclocitral; camphoreous, woody; perfuming agent; food additive	Natural Compound Flavor & Fragrance Agent Good Scents Co. Pub Chem Open Chemistry Database
214	41678-32-4	H-1-Benzopyran, 3,4,4a,5,6,8a-hexahydro	1.19	-dihydroedulan II	Research www.ChemSrc.com
215	18641-57-1	Docosanoic acid, 1,2,3-propanetriyl este	1.14	Glyceryl behenate; tribehenin; emollient, skin conditioning	Cosmetic Additive Good Scents Co. Pub Chem Open Chemistry Database
216	None	2,6-Lutidine 3,5-dichloro-4-dodecylthio-	1.14		

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#	CAS Number	Compound names of tentatively identified compounds (TICs)	Amount (ng) in 28 samples	Description	Uses/Reference
217	211563-96-1	Cyclohexene, 1,5,5-trimethyl-6-acetylmet	1.13		Research www.guidechem.com
218	3144-16-9	(+)-Camphor-10-sulfonic acid	1.12		Research Santa Cruz Biotechnology
219	None	trans-1,10-Dimethyl-trans-9-decalinol	1.08		
220	None	trans-1,10-Dimethyl-trans-9-decalol	1.07		
221	None	Z,Z,Z-4,6,9-Nonadecatriene	1.04		
222	26232-98-42	Pentene, 4,4-dimethyl-	1.04		Research www.chemSrc.com
223	267665-20-3	(1S,4S,4aS)-1-Isopropyl-4,7-dimethyl-1,2	1.03		Research NIST

Table 2. Tentatively Identified Compounds (TICS) < 1 ng g⁻¹

#	CAS Number	Compound names of Tentatively Identified Compounds (TICS)	Amount (ng) in 28 samples
224	None	Succinic acid, but-3-yn-2-yl hexyl ester	0.96
225	489-29-2	1H-Cyclopropa[a]naphthalene, 1a,2,3,3a,4	0.96
226	61847-19-6	4a,5-Dimethyl-3-(prop-1-en-2-yl)-1,2,3,4	0.94
227	None	Fumaric acid, 2-methylcyclohex-1-enylmet	0.94
228	150320-52-8	Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-m	0.92
229	38401-84-2	1,6-Dioxaspiro[4.4]nonane, 2-ethyl-	0.91
230	5767-82-8	5.alpha.-Pregn-16-en-20-one, 3.beta.,12.	0.90
231	None	Thiocyanic acid, 1,1,3-trimethyl-3-pheny	0.90
232	289-16-7	1,2,4-Trithiolane	0.90
233	10482-56-1	L-.alpha.-Terpineol	0.87
234	30460-92-5	Pinocarvone	0.86
235	None	(1,4-Dimethylpent-2-enyl)benzene	0.84
236	109837-85-6	13(S)-HODE methyl ester	0.78
237	13466-78-9	3-Carene	0.76
238	None	(1,4-Dimethylpent-2-enyl)benzene	0.74
239	471-77-2	1-Phenanthrenecarboxylic acid, 1,2,3,4,4	0.74
240	2111-75-3	Perillaldehyde	0.73
241	78-36-4	1,5-Dimethyl-1-vinyl-4-hexenyl butyrate	0.72
242	506-44-5	9,12,15-Octadecatrien-1-ol, (Z,Z,Z)-	0.66
243	105794-58-9	1-Heptatriacotanol	0.66
244	137-66-6	Ascorbic acid 6-palmitate	0.63
245	151-10-0	Benzene, 1,3-dimethoxy-	0.63
246	1786-08-9	2H-Pyran, 3,6-dihydro-4-methyl-2-(2-meth	0.62
247	None	Cyclohexane, 1,1,3-trimethyl-2,3-epoxy-2	0.62
248	None	4,4-Dimethyl-oct-5-enal	0.60
249	6453-60-7	Thymidine 3',5'-cyclic monophosphate	0.59
250	None	(E)-Hex-4-en-1-yl butyrate	0.58
251	29211-68-5	3-tert-Butyl-2-pyrazolin-5-one	0.58
252	41610-69-9	Ylangenol	0.57
253	6508-77-6	6-Tridecene, (Z)-	0.55
254	None	Tetrahydrofuran-2-one, 3-[2-pentenyl]-4-	0.55
255	2179-60-4	Disulfide, methyl propyl	0.53
256	39510-26-4	Spiro[4.5]decan-7-one, 1,8-dimethyl-4-(1	0.53
257	None	7-Hydroxy-17-oxo-9-cis-octadecanoic acid	0.52
258	142-82-5	Heptane	0.50
259	None	Quinoline, 3-dodecyl-2-methyl-4-[(4-meth	0.50
260	64580-52-5	Methyl n-hexyl disulfide	0.50
261	None	Propane, 2-(9-borabicyclo[3.3.1]non-9-yl	0.49
262	52300-90-0	Hexahydro-3H-1-[2'-trifluoromethyl]-6'-[0.48
263	2371-19-9	2-Heptanone, 3-methyl-	0.47
264	3208-16-0	Furan, 2-ethyl-	0.47
265	56666-48-9	Pyrrolidine, 1-(1-oxo-2,5-octadecadienyl	0.46
266	78-59-1	Isophorone	0.46

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#	CAS Number	Compound names of Tentatively Identified Compounds (TICs)	Amount (ng) in 28 samples
267	38667-10-6	3,3,5,5-Tetramethylcyclopentene	0.46
268	4466-24-4	2-n-Butyl furan	0.45
269	31681-26-2	2-Furanacetaldehyde, .alpha.-propyl-	0.45
270	None	3,5-Octanedione, 2,2,4,7-tetramethyl-	0.44
271	1540-36-9	2,4-Pentanedione, 3-butyl-	0.42
272	596-84-9	1H-Naphtho[2,1-b]pyran, 3-ethenyldodecah	0.42
273	55030-27-8	Cyclohexaneacetic acid, .alpha.-methyl-	0.41
274	25144-04-1	Cyclopentanol, 2-methyl-, trans-	0.39
275	472-65-1	1-Cyclohexene-1-ethanol, 2,6,6-trimethyl	0.35
276	100-47-0	Benzonitrile	0.33
277	1196-01-6	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-tri	0.33
278	None	i-Propyl 5,9,17-hexacosatrienoate	0.32
279	644-35-9	Phenol, 2-propyl-	0.28
280	19780-41-7	3-Ethyl-3-heptanol	0.27
281	57-08-9	Acexamic acid	0.27
282	1143-45-9	1-((1R,2R,3R)-2-(3-Isopropylfuran-2-yl)-	0.25
283	20851-55-2	4-Hepten-1-ol	0.24
284	None	3,9.beta.:14,15-Diepoxypregn-16-en-20-on	0.23
285	16631-62-2	E,Z-3-Ethylidenecyclohexene	0.22
286	20291-60-5	Hexane, 1-(methylthio)-	0.22
287	382-45-6	Androst-4-ene-3,11,17-trione	0.22
288	None	1-Deoxy-3,5-O-benzylidene-d-altritol	0.21
289	57150-46-6	Pyridine, 1,2,3,6-tetrahydro-1-(1-oxobut	0.18
290	None	Z-7-Hexadecenoic acid	0.17
291	None	Butyric acid, 2-phenyl-, 3-methylbut-2-e	0.15
292	67421-87-8	Methyl sec-butyl disulphide	0.13
293	182323-29-1	Thiophene, 2-ethynyl-5-[(trimethylsilyl)	0.10
294	None	Pyrimidino[5,4-b]isoquinolino[4,3-d]thio	0.10
295	24928-17-4	Decanoic acid, 1,1a,1b,4,4a,5,7a,7b,8,9-	0.10
296	24703-35-3	(1S,2E,6E,10R)-3,7,11,11-Tetramethylbicy	0.09
297	600-41-9	Allopregnane-3.beta.,7.alpha.,11.alpha.-	0.09
298	100-66-3	Anisole	0.08
399	4628-12-0	Dibutyl propanephosphonate	0.07
300	None	2-(Cyanomethylamino)pentanedinitrile	0.07
301	50991-13-4	1,1'-Bicyclohexyl, 2-ethyl-, trans-	0.07
302	1741-83-9	Pentane, 1-(methylthio)-	0.06
303	623-37-0	3-Hexanol	0.06
304	104-92-7	Benzene, 1-bromo-4-methoxy-	0.06
305	4951-40-0	2-Propenal, 3-(2,6,6-trimethyl-1-cyclohe	0.05
306	545-26-6	Gitoxigenin	0.05
307	None	trans-Decalin-2-one, 1-acetoxymethyl-6-b	0.04
309	574-77-6	Papaveroline	0.04
309	478931-82-7	trans-EKODE-(E)-Ib	0.02



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