

Article

Passive Sampling with Active Carbon Fibres in the Determination of Organic Pollutants in Groundwater

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Supplementary Materials

Table S1. List of contaminants detected in groundwater by ACF passive samplers.

tr, min	Compound	CAS	t.i./c.i.	Source / explanation
3.1	2-pentanone	107-87-9	t.i.	flavors, solvent, cosmetics
3.3	vinyl acetate	108-05-4	t.i.	monomer, solvent
3.3	tetrahydrofuran	109-99-9	t.i.	solvent
3.4	cis-dichloroethylene	156-59-2	t.i.	solvent, degreasing, decomposition of trichloroethene
3.5	trimethyl borate	121-43-7	t.i.	solvent, fungicide
3.5	ethyl acetate	141-78-6	t.i.	solvent, natural compound
3.6	4-butoxy-3-methyl-2-butanone	54340-94-2	t.i.	-
3.6	pyridine	110-86-1	t.i.	flavors, chemical intermediate
3.6	pyrazine	290-37-9	t.i.	natural compound, flavors
3.6	1-butanol	71-36-3	t.i.	natural compound, solvent
3.6	dimethyl disulfide	624-92-0	t.i.	solvent, food additive
3.6	2-i-propoxyethanol	109-59-1	t.i.	solvent, germicide
3.6	3-methyl-3-buten-2-one	814-78-8	t.i.	solvent, polymers
3.7	1,5-hexadiyne	628-16-0	t.i.	chemical intermediate
3.7	1,2-dimethoxyethane	110-71-4	t.i.	solvent
3.7	2-butanone	78-93-3	t.i.	solvent, ointment, cosmetics
3.8	bis(dimethylsilyl)methane	18163-84-3	t.i.	-
3.8	trimethyloxirane	5076-19-7	t.i.	chemical intermediate
3.8	3-penten-2-ol	1569-50-2	t.i.	natural compound, chemical intermediate
3.8	1,1,1-trichloroethane	71-55-6	t.i.	solvent
3.9	4-methyl-3-hexano	615-29-2	t.i.	-
3.9	methyl thiocyanate	556-64-9	t.i.	insecticide, chemical intermediate
3.9	benzene	71-43-2	c.i.	petroleum products
3.9	methyl pyruvate	600-22-6	t.i.	natural compound
3.9	3-hexanone	589-38-8	t.i.	natural compound, solvent
3.9	2,2,4-trimethyl-1,3-dioxolane	1193-11-9	t.i.	processing of petroleum products
3.9	1,4-dioxane	123-91-1	t.i.	stabilizer in halogenated solvents, solvent, wetting agent, cleaners
3.9	propyl acetate	109-60-4	t.i.	solvent, flavors, fragrances
3.9	3-pentanone	96-22-0	t.i.	solvent, chemical intermediate
3.9	2,2-dimethoxypropane	77-76-9	t.i.	vinyl and others polymers
4	2-methyl-2-pentanol	590-36-3	t.i.	chemical intermediate
4	trichloroethylene	79-01-6	t.i.	chemical cleaning, degreasing, industrial solvent
4	2-methoxypropanol	1589-47-5	t.i.	the degradation product of antifreeze and plastic additives
4	bromodichloromethane	75-27-4	t.i.	solvent, disinfection of water
4.1	1-chloro-2-butanol	1873-25-2	t.i.	-
4.1	3-methylbutanenitrile	625-28-5	t.i.	chemical intermediate
4.1	1-nonanol	143-08-8	t.i.	cosmetics, emulsions, solvent

4.1	dimethyl sulfite	616-42-2	t.i.	natural compound
4.2	2,2-dimethoxybutane	3453-99-4	t.i.	-
4.2	2-methoxy-2-methylbutane	994-05-8	t.i.	addition to gasoline
4.2	1,1-dimethoxy-2-methylpropane	41632-89-7	t.i.	chemical intermediate
4.2	3-methoxy-3-methyl-2-butanone	36687-98-6	t.i.	natural compound
4.2	methyl butyrate	623-42-7	t.i.	natural compound, solvent, cosmetics
4.3	diisopropoxymethane	2568-89-0	t.i.	-
4.3	2,4,5-trimethyl-1,3-dioxolane	3299-32-9	t.i.	natural compound, chemical intermediate
4.3	1,1,2-trichloroethane	79-00-5	t.i.	solvent, chemical intermediate
4.3	2-methylpyridine	109-06-8	t.i.	solvent, chemical intermediate
4.3	N-methylformamide	123-39-7	t.i.	solvent, chemical intermediate
4.4	4,4'-Oxybis(2-pentene)	52867-34-2	t.i.	-
4.4	2-butyl-4-methyl-1,3-dioxolane	74094-60-3	t.i.	flavors, fragrances
4.4	toluene	108-88-3	c.i.	petroleum products
4.4	2-methyl-3-penten-1-ol	62238-37-3	t.i.	natural compound
4.4	2-methyl butyraldehyde	96-17-3	t.i.	natural compound, food
4.4	2-methyl pyrazine	109-08-0	t.i.	incineration and pyrolysis of organic material
4.4	2-butoxy-1-methylethyl acetate	85409-76-3	t.i.	solvent
4.4	2,4-dimethyl-3-pentanone	565-80-0	t.i.	solvent
4.4	2,3-dimethyl-2-butanol	594-60-5	t.i.	solvent, chemical intermediate
4.4	methyl isobutyl ketone	108-10-1	t.i.	solvent, natural compound
4.5	2-methyloct-2-en-4-one	19860-71-0	t.i.	-
4.5	2-hexanol	626-93-7	t.i.	flavors, fragrances
4.5	2-ethyl-4-methyl-1,3-dioxolane	4359-46-0	t.i.	plastic
4.5	dibromochloromethane	124-48-1	t.i.	solvent, chemical intermediate
4.5	dimethyl sulfoxide	67-68-5	t.i.	solvent, chemical intermediate
4.5	octane	111-65-9	t.i.	solvent, chemical intermediate
4.6	1-methoxy-2-methyl-2-propanol	3587-64-2	t.i.	natural compound
4.6	2,3-dimethoxy-2-methylbutane	74421-00-4	t.i.	-
4.6	2-methyl-1,3,6-trioxocane	2781-01-3	t.i.	-
4.6	vinyl methacrylate	4245-37-8	t.i.	chemical intermediate
4.6	tetrachloroethylene	127-18-4	c.i.	chemical cleaning, degreasing, industrial solvent
4.6	2,5-dimethyl-1,4-dioxane	15176-21-3	t.i.	plastic
4.6	dimethyl oxalate	553-90-2	t.i.	the degradation product of halogenated pesticides
4.6	1-ethoxy-2-propanol	1569-02-4	t.i.	solvent, chemical intermediate
4.7	3-methyl-3-hexanol	597-96-6	t.i.	chemical intermediate
4.8	diacetone alcohol	123-42-2	t.i.	plastic additive, solvent, chemical intermediate
4.8	furfural	98-01-1	t.i.	polymers, flavors, solvent
4.8	4,4-dimethyl-2-pentanone	590-50-1	t.i.	solvent
4.8	3-methyl pyridine	108-99-6	t.i.	solvent, resins
4.9	2,2-dimethyl-3-hexanol	4209-90-9	t.i.	-
4.9	1,3-dimethoxypropane	17081-21-9	t.i.	plastic additive, antifreeze, solvent
4.9	3-hexen-1-ol	544-12-7	t.i.	cosmetics, natural compound
4.9	1,3-dioxane	505-22-6	t.i.	monomer for acetyl polymers
4.9	1-methoxy-2-propanyl acetate	108-65-6	t.i.	plasticizer
5	4,5-diamino-6-hydroxypyrimidine	1672-50-0	t.i.	-
5	1-hexanol	111-27-3	t.i.	flavors, solvent, chemical intermediate
5	methyl 3-amino-2-thiophenecarboxylate	22288-78-4	t.i.	pharmaceutical intermediate
5	butyric acid	107-92-6	t.i.	chemical intermediate, flavors, cosmetics
5	ethylbenzene	100-41-4	c.i.	oil, solvent
5	1-(1-ethoxyethoxy)propane	20680-10-8	t.i.	plastic, solvent
5	2-hexanone	591-78-6	t.i.	solvent in various preparations, ointments and antifreeze
5	t-butanol	75-65-0	t.i.	solvent, gasoline additive, pharmaceutical
5	4-methyl-3-penten-2-one	141-79-7	t.i.	solvent, resin additive
5.1	2-hydroxy-2,4-dimethyl-3-pentanone	3212-67-7	t.i.	-

5.1	ethyl dimethylcarbamate	687-48-9	t.i.	-
5.1	3-methyl-2-thiophene carboxaldehyde	5834-16-2	t.i.	flavors, natural compound
5.1	hexanenitrile	628-73-9	t.i.	burning and pyrolysis of organic material
5.1	m- + p-Xylene	108-38-3 and 106-42-3	c.i.	petroleum products, chemical intermediate
5.1	4-methyl-2-pentanol	108-11-2	t.i.	natural compound
5.2	5-methyl-3-hexanone	623-56-3	t.i.	-
5.2	2,4-dimethyl thiazole	541-58-2	t.i.	flavors, pharmaceutical intermediate
5.2	3,3-dimethyl-2-butanone	75-97-8	t.i.	chemical intermediate
5.2	phenylacetylene	536-74-3	t.i.	chemical intermediate
5.2	2,6-dimethyl heptane	1072-05-5	t.i.	natural compound
5.2	1-nonene	124-11-8	t.i.	natural compound, gasoline, chemical intermediate
5.2	n-butyl acetate	123-86-4	t.i.	solvent, flavors
5.3	dimethoxymethane	109-87-5	t.i.	cosmetics, solvent, fuel additive
5.3	o-xylene	95-47-6	c.i.	petroleum products, chemical intermediate
5.3	tribromomethane	75-25-2	t.i.	solvent, disinfection of water
5.3	2-butenic acid	3724-65-0	t.i.	solvent, additive for general use preparations
5.3	3-heptanol	589-82-2	t.i.	solvent, chemical intermediate
5.4	5,10-undecadien-3-amine	66889-12-1	t.i.	-
5.4	2-ethyl-5-methyl-1,3-dioxane	20627-54-7	t.i.	-
5.4	3,3-dimethyl-1,2-butanediol	59562-82-2	t.i.	-
5.4	2-acetylfuran	1192-62-7	t.i.	flavors, fragrances
5.4	2-decen-1-ol	22104-80-9	t.i.	flavors, fragrances
5.4	bis(methylthio)methane	1618-26-4	t.i.	flue gases, a product of microbiological processes
5.4	2-methyl cyclopentanone	1120-72-5	t.i.	chemical intermediate
5.4	2-methyl-2-cyclopenten-1-one	1120-73-6	t.i.	natural compound, food
5.4	1-ethoxybutane	628-81-9	t.i.	oxygenate
5.4	2,6-dimethyl-1,4-dioxane	10138-17-7	t.i.	plastic
5.4	1-vinyl-2-pyrrolidinone	88-12-0	t.i.	polymers, cosmetics and pharmaceuticals
5.4	2,5-dimethylpyrazine	123-32-0	t.i.	protein decomposition
5.5	2,5-dipropyltetrahydrofuran	4457-62-9	t.i.	-
5.5	4-methoxy-okt-2-en	*NIST1850 62	t.i.	-
5.5	2-aminocyclohexanol	6850-38-0	t.i.	chemical intermediate
5.5	dimethyl malonate	108-59-8	t.i.	chemical intermediate
5.5	anisole	100-66-3	t.i.	cosmetics, chemical intermediate
5.5	1,1,2,2-tetrachloroethane	79-34-5	t.i.	solvent, degreasing
5.6	6-methyl-2-octyl- (2-cis) -1,3-dioxan-4-one	99902-25-7	t.i.	-
5.6	N,N-diethylpent-2-yn-1-amine	73117-10-9	t.i.	-
5.6	2-methyl dioxane	626-68-6	t.i.	natural compound
5.6	2-methylbutyric acid	116-53-0	t.i.	natural compound, cosmetics
5.6	4-methyl-2-pentyl-1,3-dioxolan	1599-49-1	t.i.	plastic
5.6	5,5-dimethyl-1,3-dioxane	872-98-0	t.i.	plastic
5.6	2-ethylhexanal	123-05-7	t.i.	plastic
5.6	methapyrilene	91-80-5	t.i.	pharmaceuticals
5.7	N,N-diethylformamide	617-84-5	t.i.	chemical intermediate
5.7	3-penten-1-ol	39161-19-8	t.i.	natural compound, flavors, cosmetics
5.7	5-methyl-1-hepten-4-ol	99328-46-8	t.i.	natural compound, cosmetics
5.7	1-butoxypropan-2-ol	5131-66-8	t.i.	plastic, solvent
5.7	N-ethylpentanamide	54007-33-9	t.i.	tobacco smoke
5.7	3-ethyl-3-pentanol	597-49-9	t.i.	solvent
5.7	diethylene glycol dimethyl ether	111-96-6	t.i.	solvent, chemical intermediate
5.7	1-butoxypropan-2-ol	5131-66-8	t.i.	solvent, general purpose chemicals

5.7	2-butoxyethanol	111-76-2	t.i.	brake fluids, solvent
5.8	5-methyl-5-nonanol	33933-78-7	t.i.	-
5.8	2-butenic acid	503-64-0	t.i.	chemical intermediate, solvent
5.8	1-tert-butoxy-2-methoxyethane	66728-50-5	t.i.	solvent, plasticizer
5.9	1-propanone,1-(3-cyclohexen-1-yl)-2,2-dimethy	16076-65-6	t.i.	-
5.9	diethylene glycol	111-46-6	t.i.	antifreeze, cosmetics, solvent, chemical intermediate
5.9	N-ethylmorpholine	100-74-3	t.i.	chemical intermediate
5.9	2-ethyltoluene	611-14-3	t.i.	petroleum products
5.9	1-(1-methyl-2-cyclopentenyl)ethanone	68752-16-9	t.i.	natural compound
5.9	propylbenzene	103-65-1	t.i.	component of asphalt, oil
5.9	cis-2-Methylcyclohexanol	7443-70-1	t.i.	solvent, chemical intermediate
5.9	acetaldehyde ethyl methyl acetal	10471-14-4	t.i.	-
6	tetrahydro-2,5-dimethyl-2H-pyranmethanol	54004-46-5	t.i.	-
6	diisobutoxymethane	2568-91-4	t.i.	-
6	3-heptanone	106-35-4	t.i.	flavors, solvent for varnishes, cellulose, vinyl and nitrocellulose resins
6	dimethylaminoethyl acrylate	2439-35-2	t.i.	chemical intermediate, polymers
6	benzaldehyde	100-52-7	t.i.	chemical intermediate, solvent, repellent for bees
6	4-methyl valeric acid	646-07-1	t.i.	natural compound, biomass degradation
6	styrene	100-42-5	c.i.	plastic, tire, solvent, chemical intermediate
6	diisobutyl ketone	108-83-8	t.i.	solvent
6	cyclohexanol	108-93-0	t.i.	solvent, chemical intermediate
6	acetamide	60-35-5	t.i.	solvent, plasticizer, chemical intermediate
6.1	2-ethyl-1,3-dioxolane-4-methanol	53951-44-3	t.i.	-
6.1	dimethyl trisulfide	3658-80-8	t.i.	flavors, fragrances
6.1	fenole	108-95-2	c.i.	disinfection, chemical intermediate
6.1	4H-pyran-4-one	108-97-4	t.i.	product of burning
6.1	tetramethyl urea	632-22-4	t.i.	solvent
6.2	4-ethyl-2-methyl thiazole	32272-48-3	t.i.	flavors
6.2	2,4,5-trimethyl thiazole	13623-11-5	t.i.	flavors, food additive
6.2	benzonitrile	100-47-0	t.i.	cosmetics, chemical intermediate
6.2	2,2,4,6,6-pentamethylheptane	13475-82-6	t.i.	petroleum products
6.2	2-pentylfuran	3777-69-3	t.i.	natural compound, flavors
6.2	cyclohexanone	108-94-1	t.i.	production of nylon, solvent
6.2	2-butoxyethanol	111-76-2	t.i.	water-based coating solvent, component of brake fluids
6.3	glicerine	56-81-5	t.i.	cosmetics, pharmaceuticals
6.3	benzofuran	271-89-6	t.i.	coal tar
6.4	S-methyldimethylthiocarbamate	3013-02-03	t.i.	-
6.4	2,2,4-trimethylpentanenitrile	69462-10-8	t.i.	-
6.4	2-(methylamino)ethanethiol	52288-89-8	t.i.	-
6.4	tert-butyl 3-hydroxybutanoate	90435-23-7	t.i.	-
6.4	3,5,5-trimethyl hexanol	3452-97-9	t.i.	chemical intermediate
6.4	5-methyl-3-hexanol,	623-55-2	t.i.	natural compound
6.4	p-benzoquinone	106-51-4	t.i.	product of disinfection
6.4	3-octanol	589-98-0	t.i.	product of microorganisms
6.4	3-methoxypyridine	7295-76-3	t.i.	pyrolysis product
6.4	2-(2-ethoxyethoxy)-2-methylpropane	51422-54-9	t.i.	solvent
6.4	2-(2-methoxypropoxy)propan-1-ol	13588-28-8	t.i.	solvent, emulsifier
6.5	3-(2-methoxypropoxy)-1-butyne	55702-66-4	t.i.	-
6.5	2-ethyl-4,6-dimethyltetrahydropyran	*NIST 210775	t.i.	-
6.5	methyl-p-benzoquinone	553-97-9	t.i.	-
6.5	glycidyl hexyl ether	5926-90-9	t.i.	-
6.5	2-pentenoic acid	626-98-2	t.i.	flavors, natural compound

6.5	cumene	98-82-8	t.i.	addition to gasoline, chemical intermediate, solvent
6.5	1,3-dichlorobenzene	541-73-1	c.i.	insecticide, chemical intermediate
6.5	1,4-dichlorobenzene	106-46-7	c.i.	insecticide, chemical intermediate
6.5	verbenol	473-67-6	t.i.	metabolite of terpenes
6.5	isopropyl disulfide	4253-89-8	t.i.	natural compound, flavors
6.5	1-(2-methoxypropoxy)propan-2-ol	13429-07-7	t.i.	solvent, emulsifier
6.6	4,4,5-trimethyl-1,3-dioxan-5-ol	54063-14-8	t.i.	fragrances
6.6	5,5-dimethyl-2(5H)-furanone	20019-64-1	t.i.	addition of rubber
6.6	dipropylene Glycol	110-98-5	t.i.	plastic additive, solvent, air disinfection
6.6	alpha-pinene	80-56-8	t.i.	insecticide, cosmetics, solvent, plasticizers
6.6	2-ethylhexanol	104-76-7	t.i.	ointments, solvent, plasticizer
6.6	3-ethoxy-1,2-propanediol	1874-62-0	t.i.	microbial degradation of glycol ethers
6.6	2-propyl-1-pentanol	58175-57-8	t.i.	natural compound, cosmetics
6.7	(methoxymethyl)thiirane	19858-14-1	t.i.	-
6.7	3-ethylheptan-3-ol	19780-41-7	t.i.	-
6.7	2,2-dimethyl-1,3-propanediol	126-30-7	t.i.	chemical intermediate
6.7	dicyclopentadiene	77-73-6	t.i.	chemical intermediate, repellents
6.7	benzyl alcohol	100-51-6	t.i.	cosmetics, chemical intermediate
6.7	indan	496-11-7	t.i.	petroleum products
6.7	paraldehyde	123-63-7	t.i.	solvent, pharmaceutical, chemical intermediate
6.7	metaldehyde	108-62-3	t.i.	snail suppression, polymers
6.8	2,2-dimethylpropane-1-thiol	1679-08-9	t.i.	-
6.8	glycinglycine ethyl ester	627-74-7	t.i.	-
6.8	2-methylcyclohexanol	583-59-5	t.i.	flavors
6.8	butyl hexanoate	626-82-4	t.i.	flavors
6.8	o-vinyltoluene	611-15-4	t.i.	petroleum products, chemical intermediate
6.8	2-methyl-2,4-pentanediol	107-41-5	t.i.	natural compound, flavors, cosmetics
6.8	2-isopropyl-1,3-dioxolane	822-83-3	t.i.	oxygenate
6.8	1-methyl-2-pyrrolidone	872-50-4	t.i.	solvent, colors
6.8	2,2'-oxydipropanol	108-61-2	t.i.	solvent, plastic additive
6.9	p-menthan-4-ol	470-65-5	t.i.	-
6.9	3,3,5-trimethylcyclohexanone	873-94-9	t.i.	flavors
6.9	2,5-dimethyl-2,5-hexanediol	110-03-2	t.i.	chemical intermediate
6.9	4-butoxybutan-1-ol	4161-24-4	t.i.	chemical intermediate
6.9	3,7-dimethyloctan-3-ol	78-69-3	t.i.	cosmetics, natural compound
6.9	ethyl 3-hydroxyhexanoate	2305-25-1	t.i.	natural compound, food additive
6.9	2,6-Dimethyl-4-heptanone	108-83-8	t.i.	solvent, addition to polymers
6.9	2,2,5,5-tetramethyl tetrahydrofuran	15045-43-9	t.i.	solvent, chemical intermediate
6.9	2-methyl cyclohexanone	583-60-8	t.i.	solvent, rust remover
7	1-desoxy-d-mannitol	60965-81-3	t.i.	-
7	3-octanone	106-68-3	t.i.	flavors, industrial solvent also for resins and varnishes
7	decyl isobutyrate	5454-22-8	t.i.	flavors, natural compound
7	beta-pinene	127-91-3	t.i.	insecticide, solvent, plasticizer, cosmetics, chemical intermediate
7	hexanedinitrile	111-69-3	t.i.	chemical intermediate
7	4-methylbenzaldehyde	104-87-0	t.i.	cosmetics, flavors
7	methyl heptenone	110-93-0	t.i.	natural compound
7	dibutoxymethane	2568-90-3	t.i.	solvent
7	diisobutyl Ether	628-55-7	t.i.	solvent
7	1,4-diethyl benzene	105-05-5	t.i.	solvent, chemical intermediate
7	4,6-dimethylheptan-2-one	19549-80-5	t.i.	solvent, chemical intermediate, addition to polymers
7	cresol	1319-77-3	t.i.	solvent, organic intermediate, wood protection

7.1	1,4-dimethoxy-2,3-butanediol	119613-19-3	t.i.	-
7.1	N-(sulfinylamino)aniline	17420-03-0	t.i.	-
7.1	1,1,4,4-tetrachlorobutadiene	36038-53-6	t.i.	industrial chemical
7.1	acetophenone	98-86-2	t.i.	cosmetics and others
7.1	3,3,5-Trimethylcyclohexanol	116-02-9	t.i.	menthol substitute, antifoam, hydraulic fluids, esterification reagent, inks, wax additive
7.1	2-methyl-2-(methylamino)propan-1-ol	27646-73-7	t.i.	natural compound
7.1	isopropyl propyl disulphide	33672-51-4	t.i.	natural compound, flavors
7.1	methyl-propyl sulfoxide	14094-08-7	t.i.	textile industry
7.1	diethylene glycol diethyl ether	112-36-7	t.i.	solvent
7.1	2,6-dimethyl-4-heptanol	108-82-7	t.i.	solvent, addition to polymers, flavors
7.1	N-nitrosomorpholine	59-89-2	t.i.	solvent, chemical intermediate
7.2	cis-3-hexenyl Acetate	3681-71-8	t.i.	flavors, fragrances
7.2	octanal	124-13-0	t.i.	flavors, cosmetics
7.2	o-cresol	95-48-7	t.i.	disinfection, solvent, chemical intermediate
7.2	m-Cresol	108-39-4	t.i.	disinfection, solvent, chemical intermediate
7.2	cyclohexyl isocyanate	3173-53-3	t.i.	chemical intermediate
7.2	2-methylglutaronitrile	4553-62-2	t.i.	chemical intermediate, solvent
7.2	cis-homomenthol	933-48-2	t.i.	metabolite
7.3	3-isopropyl-2-phenyl-penten-2-ol	344332-17-8	t.i.	-
7.3	para-alpha-dimethyl styrene	1195-32-0	t.i.	flavors, fragrances
7.3	1-methoxy-1-methylethyl benzene	935-67-1	t.i.	flavors, cosmetics
7.3	1-(2-methoxy-1-methylethoxy)propan-2-ol	20324-32-7	t.i.	general purpose chemical
7.3	nitrobenzene	98-95-3	t.i.	solvent, chemical intermediate
7.4	1,4-diethoxy-2-butene	7250-85-3	t.i.	-
7.4	ocimene	29714-87-2	t.i.	flavors, fragrances
7.4	undecane	1120-21-4	t.i.	gasoline and other petroleum fuels
7.4	2-phenylpropan-2-ol	617-94-7	t.i.	chemical intermediate, solvent
7.4	4-cyano-1-cyclohexene	100-45-8	t.i.	bromobenzene metabolite
7.4	3,3-diethylpentane	1067-20-5	t.i.	petroleum products
7.5	1-ethyl-2-methylpyrrolidine	765-79-7	t.i.	-
7.5	2,6-dimethyl-2,5-heptadien-4-one	504-20-1	t.i.	-
7.5	D-limonene	5989-27-5	t.i.	fragrances, cosmetics
7.5	5 methyl 3 heptyne	63922-44-1	t.i.	chemical intermediate
7.5	2-methoxycyclohexanone	7429-44-9	t.i.	cosmetics
7.5	D-fenchone	126-21-6	t.i.	natural terpene compound
7.5	4-ethenyl-1,2-dimethyl-benzene	27831-13-6	t.i.	general pollutant
7.6	(E)-(3,3-dimethylcyclohexylidene)acetaldehyde	26532-25-2	t.i.	-
7.6	2-propyl-1,3-dioxonane	*NIST 249774	t.i.	-
7.6	dihydrocarveol	619-01-2	t.i.	flavors, fragrances
7.6	2,2'-azobis(isobutyronitrile)	78-67-1	t.i.	plastic additive
7.6	methyl octanoate	111-11-5	t.i.	chemical intermediate, food additive
7.6	triethyl phosphate	78-40-0	t.i.	plasticizer
7.6	2-methyloctan-1-ol	818-81-5	t.i.	solvent
7.7	4-acetylocta-1,2-diene	*NIST 250445	t.i.	-
7.7	alpha-hydroxy-alpha-methylbenzyl phenyl ketone	5623-26-7	t.i.	-
7.7	4,6-dimethyl-2-pyrone	675-09-2	t.i.	fragrances
7.7	tempidon	826-36-8	t.i.	chemical intermediate
7.7	N-formylmorpholine	4394-85-8	t.i.	solvent
7.8	1-ethylpyrrolidin-2-one	2687-91-4	t.i.	chemical intermediate
7.8	beta-pinone	24903-95-5	t.i.	natural compound

7.8	3,4-dimethylhexane-2,5-dione	25234-79-1	t.i.	plastic
7.8	N,2-dimethylpropanamide	2675-88-9	t.i.	tobacco smoke, chemical intermediate
7.8	N-isobutyl acetamide	1540-94-9	t.i.	tobacco smoke, food
7.9	4,6-decadiyne	16387-71-6	t.i.	-
7.9	4H-1,3-benzodioxin	254-27-3	t.i.	-
7.9	N-isoamyl acetamide	13434-12-3	t.i.	-
7.9	1,2-dimethoxybenzene	91-16-7	t.i.	flavors
7.9	1-[1-methyl-2-(2-propenyloxy)ethoxy]-2-propanol	55956-25-7	t.i.	color additive
7.9	(1r)-(+)-nopinone	38651-65-9	t.i.	natural compound
7.9	1-octanol	111-87-5	t.i.	solvent, cosmetics
8	3,5,5-trimethylhexanoic acid	3302-10-1	t.i.	chemical intermediate
8	3-ethyle-4-nonanol	19780-72-4	t.i.	-
8	2-methylbenzaldehyde	529-20-4	t.i.	exhaust gases
8	but-3-en-2-ylbenzene	934-10-1	t.i.	petroleum products
8	2,4-dimethyl styrene	2234-20-0	t.i.	petroleum products, chemical intermediate, component of gum
8	4-methylindan	824-22-6	t.i.	decomposition of petroleum products
8.1	2-ethyl thiazolidine	24050-09-7	t.i.	-
8.1	diethyl ethylphosphonate	78-38-6	t.i.	addition to gasoline, plasticizer, textile processing
8.1	2-phenylacetamide	103-81-1	t.i.	pharmaceutical intermediate, metabolite
8.1	2,2,6,6-tetramethylpiperidin-4-ol	2403-88-5	t.i.	chemical intermediate
8.1	2,6-dimethylaniline	87-62-7	t.i.	chemical intermediate
8.1	dimethyl benzyl carbinol	100-86-7	t.i.	cosmetics, natural compound
8.1	3-methyl undecane	1002-43-3	t.i.	petroleum products
8.1	sabina ketone	513-20-2	t.i.	natural compound, cosmetics
8.2	tert-butyl cyclohexanecarboxylate	16537-05-6	t.i.	-
8.2	2,4,6-trimethyl-decane	62108-27-4	t.i.	-
8.2	2-hexyl-1-n-octanol	19780-79-1	t.i.	-
8.2	dibutyltin dilaurate	88481-58-7	t.i.	-
8.2	p-cresol	106-44-5	t.i.	disinfection, solvent, chemical intermediate
8.2	1,2,3-trimethylindene	4773-83-5	t.i.	petroleum products
8.2	1,3-Dimethoxybenzene	151-10-0	t.i.	natural compound, flavors, cosmetics
8.2	2-propylheptan-1-ol	10042-59-8	t.i.	component of petroleum products, waste water
8.2	o-cymene	527-84-4	t.i.	solvent, chemical intermediate
8.3	2-methyl-1-hexene	6094-02-6	t.i.	-
8.3	3-methyl-1- (methylsulfinyl) butane	55860-10-1	t.i.	-
8.3	nonanal	124-19-6	t.i.	flavors, cosmetics
8.3	2-(2-butoxyethoxy)ethanol	112-34-5	t.i.	solvent, chemical intermediate
8.3	1,2,3,4-tetrahydronaphthalene	119-64-2	t.i.	solvent, decomposition of petroleum products
8.3	2-(2-ethoxyethoxy)ethanol	111-90-0	t.i.	solvent, brake fluids, cosmetics
8.4	1,2-dihydro-8-hydroxylinalol	*NIST 131835	t.i.	-
8.4	2,4-dimethyl-pentane-2,3-diol	66225-53-4	t.i.	-
8.4	bicyclo[2.2.2]octane-1,4-diol	1194-44-1	t.i.	-
8.4	2,2,6,6-tetramethyl-4-piperidone	826-36-8	t.i.	alkaloide
8.4	4-acetylmorpholine	1696-20-4	t.i.	chemical intermediate
8.4	tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one	7226-23-5	t.i.	chemical intermediate
8.4	methyl benzoate	93-58-3	t.i.	cosmetics
8.4	dextro-dihydrocarvone	7764-50-3	t.i.	cosmetics, natural compound
8.4	dimethyl trithiocarbonate	2314-48-9	t.i.	microbiological processes
8.4	p-cimen-8-ol	1197-01-9	t.i.	natural compound, biomass degradation, flavors
8.5	1,7,7-trimethylbicyclo [2.2.1] heptane-2,5-diol	10359-41-8	t.i.	-
8.5	2-piperidone	675-20-7	t.i.	pharmaceutical intermediate
8.5	N,N'-dimethylparabanic acid	5176-82-9	t.i.	metabolite of caffeine

8.5	2-methyl-2H-benzotriazole	16584-00-2	c.i.	anti-corrosion agents, herbicidal and antimicrobial preparations
8.5	4,7-dimethylindan	6682-71-9	t.i.	tobacco smoke
8.5	sulfolane	126-33-0	t.i.	solvent, resins
8.6	1-methyl-4- (1-methyl-2-propenyl) benzene	97664-18-1	t.i.	-
8.6	4-ethoxycyclohexanone	23510-92-1	t.i.	-
8.6	naphthalene	91-20-3	c.i.	chemical intermediate, constituent of moth repellents
8.6	2,4,8,10-tetraoxaspiro[5.5]undecane	126-54-5	t.i.	chemical intermediate
8.6	2-[(2-ethylhexyl)oxy]ethanol	1559-35-9	t.i.	chemical intermediate, solvent, colors
8.6	2-phenylethyl alcohol	60-12-8	t.i.	general purpose chemical, natural compound
8.6	phenoxyacetone	621-87-4	t.i.	general purpose chemical, waste water
8.6	1-i-propenyl-3-i-propylbenzene	1129-29-9	t.i.	petroleum products
8.6	6-metil-1-okten	13151-10-5	t.i.	petroleum products
8.6	6-methyl-1-octene	110453-78-6	t.i.	natural compound, cosmetics
8.6	2-methyl valeric acid	97-61-0	t.i.	natural compound, biomass degradation
8.6	1,3,5,7-tetroxocane	293-30-1	t.i.	formaldehyde tetramer
8.6	1-butoxyethoxy-2-propanol	124-16-3	t.i.	solvent, chemical intermediate
8.7	2-thio-2,4-oxazolidinedione	2346-24-9	t.i.	-
8.7	5-methyl isoxazolidinone	41833-03-8	t.i.	-
8.7	6,7-dimethyl dihydrocyclopentapyrazine	38917-61-2	t.i.	flavors
8.7	2',4'-dimethyl acetophenone	89-74-7	t.i.	flavors, cosmetics
8.7	octaethyleneglycol monododecyl ether	3055-98-9	t.i.	detergent
8.7	cyclohexyl isothiocyanate	1122-82-3	t.i.	tire, industrial wastewater
8.7	2,5-dimethyl-1H-benzimidazole	1792-41-2	t.i.	chemical intermediate
8.7	dimethyltetrasulfide	5756-24-1	t.i.	microbiological processes
8.7	1,3-diisopropylbenzene	99-62-7	t.i.	petroleum products
8.7	3-ethyl-4-methyl-pyrrole-2,5-dione	20189-42-8	t.i.	natural compound, flavors, waste water
8.7	2,6-dichloroaniline	608-31-1	t.i.	Diclofenac (pharmaceutical) oxidation
8.7	1,2-bis(2-methoxyethoxy)ethane	112-49-2	t.i.	solvent, plasticizer
8.8	1,3-di-tert-butylbenzene	1014-60-4	t.i.	-
8.8	1-phenyl-1-butene	824-90-8	t.i.	-
8.8	2,3-dimethoxytoluene	4463-33-6	t.i.	flavors
8.8	benzothiazole	95-16-9	t.i.	addition of rubber, antimicrobial preparations, flavors
8.8	N,N-dimethylmethanesulfonamide	918-05-8	t.i.	chemical intermediate
8.8	2,5-dimethyl benzoxazole	5676-58-4	t.i.	natural compound
8.9	tropine 4-tolylacetate methiodide	5135-79-5	t.i.	-
8.9	4-methoxymethoxy-2-methyl-butan-2-ol	37587-78-3	t.i.	-
8.9	2-propylcyclohexanone	94-65-5	t.i.	-
8.9	2-tert-butyl-1,4-benzoquinone	3602-55-9	t.i.	antioxidant
8.9	hydroxyciol	107-74-4	t.i.	flavors
8.9	1-methyltetraline	1559-81-5	t.i.	atmospheric reactions
8.9	D-sorbitol	50-70-4	t.i.	food, cosmetics
8.9	2,4-dichloroaniline	554-00-7	t.i.	chemical intermediate
8.9	1,2-octanediol	1117-86-8	t.i.	cosmetics, pharmacy
8.9	4-hydroxy-3-methyl acetophenone	876-02-8	t.i.	natural compound
8.9	desulphosinigrin	5115-81-1	t.i.	natural compound
8.9	(E)-2-decenal	3913-81-3	t.i.	natural compound, cosmetics
8.9	4-isopropylphenyl isocyanate	31027-31-3	t.i.	thermal decomposition of isoproturon herbicides
8.9	tetraethylene glycol diethyl ether	4353-28-0	t.i.	solvent, plasticizer
9	3,3'-oxydipropionitrile	1656-48-0	t.i.	chemical intermediate
9	benzoic acid	65-85-0	t.i.	chemical intermediate
9	methyl 3-hydroxyoctanoate	7367-87-5	t.i.	natural compound
9	methyl phenyl acetate	101-41-7	t.i.	natural compound, flavors

9	3-ethoxyphenol	621-34-1	t.i.	the degradation product of anisole, natural compound
9	octanoic acid	124-07-2	t.i.	disinfectant, synthesis of dyes, perfumes
9	1-phenoxy-2-propanol	770-35-4	t.i.	solvent, cosmetics
9.1	o-i-propoxyphenyl methylcarbamate	114-26-1	t.i.	insecticide
9.1	2-ethyl-2,3-dihydro-1H-indene	56147-63-8	t.i.	-
9.1	undecanoic acid	112-37-8	t.i.	flavors
9.1	nonanoic acid	112-05-0	t.i.	herbicidal formulations, disinfectant, cosmetics
9.1	3,3,4,4-tetramethylsuccinimide	3566-61-8	t.i.	chemical intermediate
9.1	1-decanol	112-30-1	t.i.	cosmetics, chemical intermediates, additive to plasticizers
9.1	4,4-dimethyl-1,3-dioxane	766-15-4	t.i.	plastic
9.1	caprolactam	105-60-2	t.i.	polyamide fibers
9.1	2-propoxyphenol	6280-96-2	t.i.	solvent
9.2	D-trans-1,2,2,3-tetramethylcyclopentane carboxylic acid	31147-56-5	t.i.	-
9.2	2-methyl-5-isopropylcyclohexanol	60320-28-7	t.i.	-
9.2	3-hydroxydodecanoic acid	1883-13-2	t.i.	-
9.2	N,N-diethylbutylamine	4444-68-2	t.i.	-
9.2	neocarvomenthol	1126-40-5	t.i.	-
9.2	delta-decalactone	705-86-2	t.i.	flavors, fragrances
9.2	triisopropyl phosphate	513-02-0	t.i.	plastic additive
9.2	1,3-diisopropenylbenzene	3748-13-8	t.i.	petroleum products
9.2	dodecane	112-40-3	t.i.	petroleum products
9.3	1,2,3,4,5-pentamethylcyclopentane	*NIST 152797	t.i.	-
9.3	karvomenton	499-70-7	t.i.	flavors, fragrances
9.3	3-methylcaprolactam	2073-32-7	t.i.	-
9.3	ethyl 2-methoxyimino-4-oxopentanoate	82874-96-2	t.i.	-
9.3	decanal	112-31-2	t.i.	flavors, cosmetics
9.3	dimethyl methylcarbonodithioimide	18805-25-9	t.i.	pharmaceutical
9.3	2,4-dimethyl-2H-benzotriazole	-	t.i.	herbicidal and antimicrobial preparations, decomposition of anti-corrosion preparations
9.3	methylparaben	99-76-3	t.i.	preservative in food, beverage, cosmetics
9.3	1-heptadecanol	1454-85-9	t.i.	lubricants, plasticizers
9.4	4,7-dimethyl-3a, 4,7,7a-tetrahydro-2-benzofuran-1,3-dione	2651-48-1	t.i.	-
9.4	β -Ionone	79-77-6	t.i.	flavors, fragrances
9.4	N,N-dibutylformamide	761-65-9	t.i.	solvent
9.4	trimethylolpropane	77-99-6	t.i.	chemical intermediate
9.4	indol	120-72-9	t.i.	cosmetics, chemical intermediate
9.4	undecanal	112-44-7	t.i.	cosmetics, natural compound
9.4	1-methylhydantoin	616-04-6	t.i.	metabolite of pharmaceuticals
9.4	1,2,3-benzenetricarboxylic acid	569-51-7	t.i.	a natural phenolic compound
9.4	5-Methylhydantoin	616-03-5	t.i.	natural compound, microbiological reactions
9.4	3,3a,4,6,7,7a-hexahydro-4,7-methano-5H-inden-5-one	14888-58-5	t.i.	plastic
9.4	camphor	76-22-2	t.i.	plastic, pharmaceuticals, repelent, natural compound
9.4	2-undecanol	1653-30-1	t.i.	admixture to other compounds
9.4	edulan	41678-29-9	t.i.	food
9.4	2-mercaptopyridine	2637-34-5	t.i.	pharmaceuticals
9.4	2-amino-5-nitrothiazole	121-66-4	t.i.	pharmaceuticals
9.5	1-decalone	4832-16-0	t.i.	-
9.5	N-ethyl-1,3-dimethylbutan-1-amine	42966-64-3	t.i.	-
9.5	isopropyl 4-oxovalerate	21884-26-4	t.i.	flavors

9.5	1-indanone	83-33-0	t.i.	cigarette smoke, waste water
9.5	3-tert-butylphenol	585-34-2	t.i.	pharmacy, fragrances
9.5	2-ethyl-1-butene	760-21-4	t.i.	chemical intermediate
9.5	1-(4-propan-2-ylphenyl)propan-1-ol	54518-11-5	t.i.	chemical intermediate
9.5	phenyl acetic acid	103-82-2	t.i.	natural compound, flavors
9.5	2,4-decadienal	2363-88-4	t.i.	oils, natural compound, flavors
9.5	N,N-dimethylbutan-2-amine	921-04-0	t.i.	surfactant
9.5	1,2,3-trimethoxybenzene	634-36-6	t.i.	smoked food
9.6	ethyl cyclopropanecarboxylate	4606-07-9	t.i.	-
9.6	2-hydroxypiperitone	490-03-9	t.i.	natural compound
9.6	methyl 6-methylsalicylate	33528-09-5	t.i.	-
9.6	formanilide	103-70-8	t.i.	analgesic, antipyretic
9.6	2,4,6-trichloroanisole	87-40-1	t.i.	metabolite of 2,4,6-trichlorophenol fungicide, product of mold
9.6	5-methyl-1,2,3,4-tetrahydronaphthalene	2809-64-5	t.i.	petroleum products
9.6	camphor oxime	13559-66-5	t.i.	natural compound
9.6	4,8-dimethyl-1-nonanol	33933-80-1	t.i.	natural compound, cosmetics
9.6	tripropylene glycol	1638-16-0	t.i.	solvent, chemical intermediate
9.7	n-(2,6-dimethylphenyl)formamide	607-92-1	t.i.	pharmaceutical
9.7	2,6-dihydroxybenzoic acid	303-07-1	t.i.	microbiological processes
9.7	3-decen-1-ol (Z)	10340-22-4		natural compound
9.7	2-methyl-1-indanone	17496-14-9	t.i.	tobacco smoke
9.7	3,3-dimethyl-1-indanone	26465-81-6	t.i.	pharmaceuticals
9.8	1,2-dimethyl-2,3-dihydro-1H-indole	26216-93-3	t.i.	-
9.8	N-(2,6-dimethylphenyl)acetamide	2198-53-0	t.i.	-
9.8	2,5-dihydroperoxy-2,5-dimethylhexane	3025-88-5	t.i.	addition to polymers
9.8	pinanediol	22422-34-0	t.i.	chemical intermediate
9.8	1-(4-tert-butylphenyl)ethanol	34386-42-0	t.i.	cosmetics, flavors
9.9	isopropylidenecyclohexane	5749-72-4	t.i.	-
9.9	N,N-dibutylacetamide	1563-90-2	t.i.	-
9.9	4,4'-methylenediphenyl diisocyanate	116437-28-6	t.i.	-
9.9	limonene glycol	1946-00-5	t.i.	flavors
9.9	4-hydroxybenzyl alcohol	623-05-2	t.i.	flavors
9.9	butyl octanoate	589-75-3	t.i.	flavors, fragrances
9.9	4'-isopropylacetophenone	645-13-6	t.i.	cosmetics, flavors
9.9	2-(2-butoxyethoxy)ethyl acetate	124-17-4	t.i.	solvent, plasticizer
9.9	ethinamate	126-52-3	t.i.	pharmaceuticals
10	4-(2-propenyl)acetophenone	5359-06-04	t.i.	plastic, cosmetics
10	2-(hydroxymethyl)benzoic acid	612-20-4	t.i.	-
10	2-cyclopentaneethanol	766-00-7	t.i.	-
10	phenylmalonic acid	2613-89-0	t.i.	-
10	3-hydroxybenzaldehyde	100-83-4	t.i.	food additive
10	1-isopropyl-2,2-dimethyltrimethylene diisobutyrate	6846-50-0	t.i.	plasticizer
10	3H-2-benzofuran-1-one	87-41-2	t.i.	natural compound
10.1	3,4-dimethylacetophenone	3637-01-2	t.i.	-
10.1	2',5'-dimethyl acetophenone	2142-73-6	t.i.	-
10.1	3-ethoxy-4-hydroxybenzaldehyde	4230-32-4	t.i.	-
10.1	2-hydroxybenzaldehyde	57732-90-8	t.i.	-
10.1	3-hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	74367-34-3	t.i.	-
10.1	6,10-dimethylundecan-2-one	1604-34-8	t.i.	flavors, fragrances
10.1	5-chloro-2-methylbenzoxazole	19219-99-9	t.i.	chemical intermediate
10.1	6-tridecene	24949-38-0	t.i.	petroleum products
10.1	cuminaldehyde	122-03-2	t.i.	natural compound

10.1	(Z)-rose oxide	16409-43-1	t.i.	natural compound
10.1	1-methyl-1H-benzotriazole	13351-73-0	t.i.	the degradation of 1H-benzotriazole
10.2	3-(trimethoxysilyl)-1-propanethiol	36879-74-0	t.i.	-
10.2	n-Tridecane	629-50-5	t.i.	petroleum products, solvent, chemical intermediate
10.2	4-hydroxybenzaldehyde	123-08-0	t.i.	natural compound, biomass degradation
10.3	3-fluoroacetanilide	351-28-0	t.i.	-
10.3	undecanol	112-42-5	t.i.	flavor, additives, fragrances
10.3	thymol	89-83-8	t.i.	flavors, cosmetics
10.3	2-aminoacetophenone	551-93-9	t.i.	chemical intermediate
10.3	methyl decanoate	110-42-9	t.i.	chemical intermediate
10.3	1-tetralone	529-34-0	t.i.	chemical intermediate, solvent
10.3	3,4,5-trimethoxytoluene	6443-69-2	t.i.	waste water
10.3	2,4,7,9-tetramethyldec-5-yne-4,7-diol	126-86-3	t.i.	wetting agent, FFS ingredient, antifoam, detergent ingredient
10.3	5,5-dimethyl-1,3-cyclohexanedione	126-81-8	t.i.	decay of plastics
10.4	cyclohexyl isopropyl phosphono fluoridate	333416-55-0	t.i.	-
10.4	4-isopropyl- α,α -dimethylbenzyl alcohol	3445-42-9	t.i.	-
10.4	4-tert-butylphenol	98-54-4	t.i.	plastic additive
10.4	2-methyl quinoline	91-63-4	t.i.	pharmaceutical, microbiological processes
10.4	1,3-diacetylbenzene	6781-42-6	t.i.	pharmaceutical intermediate
10.4	dodecanal	112-54-9	t.i.	cosmetics
10.4	para-tert-butyl acetophenone	943-27-1	t.i.	plastic, cosmetics
10.4	2-hydroxyethyl methacrylate	868-77-9	t.i.	polymers
10.4	benzyl benzoate	120-51-4	t.i.	repellent, fragrances, veterina
10.4	2,6-diisopropylphenol	2078-54-8	t.i.	pharmaceuticals
10.5	2-trifluoromethyl-nicotinamide	959108-47-5	t.i.	-
10.5	3-tert-butyl-5-ethyltoluene	6630-01-9	t.i.	-
10.5	allyl crotonate	20474-93-5	t.i.	flavors
10.5	vanillin	121-33-5	t.i.	flavors, cosmetics
10.5	tripropylene glycol monomethyl ether	20324-33-8	t.i.	colors, cleaners
10.5	propyl tiglate	61692-83-9	t.i.	natural compounds
10.6	4,5-diethyl-2,3-dimethyl-2,3-dihydrofuran	54244-89-2	t.i.	-
10.6	ethyl cyclopropane carboxylate	4606-07-09	t.i.	chemical intermediate
10.6	2,4-diethyl-6-methyl-1,3,5-trioxane	117888-04-7	t.i.	-
10.6	5-hydroxy-3,3,6,6-tetramethyl-4-thiepanone	4485-40-9	t.i.	-
10.6	3-(2-hydroxypropyl)-5-methyl-2-oxazolidinone	3375-84-6	t.i.	-
10.6	1,2-dihydro-2,2,4-trimethylquinoline	147-47-7	t.i.	antioxidant
10.6	2-ethylhexyl mercaptoacetate	7659-86-1	t.i.	chemical intermediate
10.6	N-(2,5-dimethylphenyl)formamid	10113-40-3	t.i.	chemical intermediate
10.6	1,4-diacetylbenzene	1009-61-6	t.i.	rubber mesh reagent
10.7	4'-isobutylacetophenone	38861-78-8	t.i.	-
10.7	4'-methylbutyrophenone	4160-52-5	t.i.	chemical intermediate
10.7	3-phenyl propionic acid	501-52-0	t.i.	chemical intermediate
10.7	dicyclohexylamine	101-83-7	t.i.	chemical intermediate, color, insecticide, anticorrosive agent, plasticizer, antioxidant
10.7	1-octadecanol	112-92-5	t.i.	cosmetics, chemical intermediate, perfumes, additives
10.7	2,2,6,7-tetramethyl-10-oxatricyclo[4.3.0.1(1,7)]decan-5-one	121747-63-5	t.i.	natural compound
10.7	geranyl acetone	689-67-8	t.i.	natural compound
10.7	1,4-dimethyl-1H-benzotriazole	-	t.i.	benzotriazoles
10.7	digitoxin	71-63-6	t.i.	pharmaceuticals

10.8	5-bromo-6-chloro-3-indolyl- β -D-	43125-89-9	t.i.	-
10.8	3,3,6-trimethylbicyclo[3.1.0]hexan-2-one	53966-40-8	t.i.	-
10.8	benzaldehyde propylene glycol acetal	2568-25-4	t.i.	flavors
10.8	4-(decyloxy)benzoic Acid	5519-23-3	t.i.	pharmaceutical
10.8	2,4-dimethylquinoline	1198-37-4	t.i.	tire, petroleum products
10.8	1,2-decanediol	1119-86-4	t.i.	chemical intermediate
10.8	3,3-dimethylphthalide	1689-09-4	t.i.	chemical intermediate
10.8	decanoic acid	334-48-5	t.i.	cosmetics, intermediat
10.8	dimethyl phthalate	131-11-3	c.i.	plasticizer, solvent
10.8	3,3-dimethyl-1,5-ditert-butyl-bicyclo[3.1.0]hexan-4-one	19377-95-8	t.i.	plastic
10.9	2,3-dimethylbenzamide	5580-34-7	t.i.	-
10.9	methyl 12-methyltetradecanoate	5129-66-8	t.i.	-
10.9	3,4-dihydro-8-methyl naphthalenone	51015-28-2	t.i.	cosmetics
10.9	1-dodecanol	112-53-8	t.i.	natural compound, flavors, cosmetics, detergents and wetting agents
10.9	2,6-di-tert-butyl-1,4-benzoquinone	719-22-2	t.i.	oxidizer, catalyst
11	(2-isothiocyanato methyl) -benzene	2257-02-09	t.i.	natural compound
11	gamma-decalactone	706-14-9	t.i.	flavors
11	dicyclopentadiene diepoxide	81-21-0	t.i.	addition of rubber, epoxy resins
11	1-[4-(2-hydroxypropan-2-yl)phenyl]ethanone	54549-72-3	t.i.	tire
11	alpha, alpha'-dihydroxy-1,3-diisopropylbenzene	1999-85-5	t.i.	chemical intermediate
11	tetradecane	629-59-4	t.i.	petroleum products
11	1H-benzotriazole	95-14-7	t.i.	anti-corrosion agents
11	undecan-4-olide	104-67-6	t.i.	repellent
11.1	6-methyl-3-(1-methylethyl)-2-oxo-1-(3-oxobutyl)	22339-30-6	t.i.	-
11.1	decyl acetate	112-17-4	t.i.	flavors
11.1	2-methylindole	95-20-5	t.i.	flavors, burning and pyrolysis of organic material
11.1	2-tridecanone	593-08-8	t.i.	natural compound, flavors, cosmetics
11.1	tetraethylene glycol dimethyl ether	143-24-8	t.i.	solvent
11.2	6-methyl-3(2H)-benzofuranone	20895-41-4	t.i.	-
11.2	butyl 2-butenate	7299-91-4	t.i.	-
11.2	(2S)-1,2,3,4-tetrahydro-8-hydroxy-4-oxoquinoline-2-carboxylic acid	4886-42-4	t.i.	-
11.2	tributyl phosphate	126-73-8	t.i.	plastic additive
11.2	2-tridecanol	1653-31-2	t.i.	natural compound
11.2	tridecanal	10486-19-8	t.i.	natural compound, cosmetics
11.2	4'-aminopropiophenone	70-69-9	t.i.	pesticide
11.3	2,5-heptadecadion	66408-88-6	t.i.	-
11.3	N-(2-phenylethyl)acetamide	877-95-2	t.i.	-
11.3	4-isopropyl-phenetole	4132-79-0	t.i.	-
11.3	3,5-diisopropyl-1,2,4-trithiolane	54934-99-5	t.i.	flavors
11.3	tetrapropylene glycol, monomethyl ether	20324-34-9	t.i.	colors, cleaners
11.3	alpha, alpha'-dihydroxy-1,4-diisopropylbenzene	2948-46-1	t.i.	plastic additive
11.3	2,6-diacetylpyridine	1129-30-2	t.i.	chemical intermediate
11.3	4-isopropylaniline	99-88-7	t.i.	degradation product of herbicide isoproturon
11.3	2-butyl-5-ethyl thiophene	54411-06-2	t.i.	synthesis of arom
11.4	N, N-dicyclohexylmethylamine	7560-83-0	t.i.	-
11.4	N-metil dicikloheksilamin	7560-83-0	t.i.	-
11.4	isobutyl tiglate	61692-84-0	t.i.	flavors, natural compound
11.4	cycluron	2163-69-1	t.i.	herbicide
11.4	3-hydroxyphenyl benzoate	136-36-7	t.i.	UV absorber
11.5	N- (4-pyridinylmethyl) -1H-indole-3-ethanamine	900350-59-2	t.i.	-

11.5	3,5-diethyl-4-imino-2,5-cyclohexadien-1-one	108451-26-9	t.i.	the degradation product of chloroacetanilide herbicides
11.5	2,2-bis(4-methoxyphenyl)acetic acid	20797-56-2		-
11.5	ethyl 4-(2-hydroxyphenyl)-2,4-dioxobutanoate	4940-37-8	t.i.	-
11.5	3-methylindole	83-34-1	t.i.	pharmacy, food additive, cosmetics
11.6	3,4-dihydro-5-methyl naphthalenone	6939-35-1	t.i.	cosmetics
11.6	4-methyl-1H-benzotriazole	29878-31-7	t.i.	de-icing agent, anti-corrosion protection, fungicide
11.7	1,2,3,4,4A, 8A-hexahydro-alpha, alpha, 4A-2-ol-lenmethanol	29484-47-7	t.i.	-
11.7	4-methyl-1-tetralone	19832-98-5	t.i.	-
11.7	1,2,4-triazine-3,5(2H,4H)-dione,6-(1,1-dimethylethyl)	52236-30-3	t.i.	-
11.7	6-ethyl-4,5-decanediol	22607-12-1	t.i.	-
11.7	ethyl 2-methyl-2-butenate	55514-48-2	t.i.	flavors, fragrances
11.7	dihydroactinidiolide	15356-74-8	t.i.	flavors, fragrances
11.7	3-tert-butyl-4-hydroxyanisole	121-00-6	t.i.	food additive
11.7	lauric acid	143-07-7	t.i.	general purpose chemical, cosmetics, , food additive
11.7	2,5-diisobutyl thiophene	54845-33-9	t.i.	cosmetics
11.7	alpha-selinene	473-13-2	t.i.	natural compound
11.7	5-hydroxyvanillin	3934-87-0	t.i.	oxidation of lignin
11.7	dihydroactinidiolide	17092-92-1	t.i.	a raw material for fragrances, a decomposition product of beta-carotene
11.8	1-(2,4,6-trihydroxyphenyl)butan-1-one	2437-62-9	t.i.	-
11.8	triethylene glycol monomethyl ether	112-35-6	t.i.	solvent, chemical intermediate, softener
11.9	4-pentadecyl ester- 2,5-difluorobenzoic acid	900338-48-1	t.i.	-
11.9	decyl isopropylphosphonofluoridoate	333416-36-7	t.i.	-
11.9	benzenesulfonamide	98-10-2	t.i.	chemical intermediate
11.9	hexadecane	544-76-3	t.i.	petroleum products, solvent
11.9	2-chloro-4,6-diamino-1,3,5-triazinen	3397-62-4	t.i.	degradation product of herbicide atrazine and propazine
11.9	2,6-dimethoxy-1,4-benzoquinone	530-55-2	t.i.	wood decomposition
12	2,3,3-trimethyl-3H-indol-5-amine	773-63-7	t.i.	pharmaceutical intermediate
12	nonadecane	629-92-5	t.i.	cosmetics, fragrances
12	isobutyl 3-methyl-2-butenate	30434-54-9	t.i.	cosmetics, natural compound
12	pentadecane	629-62-9	t.i.	petroleum products, chemical intermediate, solvent
12	diethyltoluamide	134-62-3	t.i.	repellent
12	levetiracetam	102767-28-2	t.i.	pharmaceuticals
12.1	1-methylindole-2,3-dione	64605-28-3	t.i.	-
12.1	gabapentin	60142-96-3	t.i.	analgesic
12.1	5,6-dimethyl-1,2,3-benzotriazole	4184-79-6	t.i.	anti-corrosion products, anti-icing preparations
12.1	α-murolene	10208-80-7	t.i.	flavors
12.1	1-phenylpent-1-en-3-one	3152-68-9	t.i.	natural compound
12.1	guaiol	489-86-1	t.i.	natural terpene compound
12.1	1,4,7,10,13-pentaoxacyclopentadecane	33100-27-5	t.i.	pesticides
12.2	vinyl myristate	5809-91-6	t.i.	-
12.2	methyl dodecanoate	111-82-0	t.i.	flavors, chemical intermediate
12.2	2,6-dimethylphenyl isocyanate	28556-81-2	t.i.	chemical intermediate
12.2	dodecyl acetate	112-66-3	t.i.	natural compound
12.3	p-tert-butylpivalophenone	22583-66-0	t.i.	-
12.3	3-acetamide-1-phenylpyrazole	2753-56-2	t.i.	-
12.3	4-(4-methylphenyl)-1H-1,2,3-triazole	5301-96-2	t.i.	-

12.3	4-(methylsulfonyl)aniline	5470-49-5	t.i.	-
12.3	5-ethyl-3,4-dihydro-1(2H)-naphthalenone	51015-31-7	t.i.	-
12.3	tetradecanal	124-25-4	t.i.	flavors, fragrances
12.3	3,4,5-trimethoxybenzaldehyde	86-81-7	t.i.	pharmaceutical intermediate
12.3	3,3,6,8-tetramethyl-2,4-dihydronaphthalen-1-one	5409-55-2	t.i.	petroleum products
12.3	myristyl alcohol	112-72-1	t.i.	natural compound, component of fragrances, synthesis of myristyl myristate
12.4	oxacyclotetradeca-4-11-diyne	6568-32-7	t.i.	-
12.4	dihydrojasnone	1128-08-1	t.i.	flavors, fragrances
12.4	(2-acetylphenyl) formamide	5257-06-7	t.i.	natural compound, biomass degradation
12.4	1-pentadecanol	629-76-5	t.i.	plasticizer, emulsifier
12.5	5-methyl-1H-benzotriazole	136-85-6	t.i.	anti-corrosion products
12.5	o-toluenesulfonamide	88-19-7	t.i.	plasticizer, chemical intermediate
12.6	2-acetylphenyl-formamide	900305-65-7	t.i.	-
12.6	2-butyl-5-isobutyl thiophene	54845-35-1	t.i.	-
12.6	6,7-dimethyl-1-tetralone	19550-57-3	t.i.	-
12.6	dioctyl ether	629-82-3	t.i.	chemical intermediate, plasticizer, solvent
12.6	ibuprofen	15687-27-1	t.i.	pharmaceuticals
12.7	propylene carbonate anhydrous	91143-32-7	t.i.	-
12.7	desisopropylatrazine	1007-28-9	c.i.	metabolite of atrazine
12.7	izoaromadendren epoksid	NIST159366	t.i.	natural compound
12.7	2(3H)-benzofuranone	16778-27-1	t.i.	natural terpenoid compound
12.7	diethylene glycol dimethacrylate	2358-84-1	t.i.	plastic
12.8	benzophenone	119-61-9	t.i.	fragrances, UV absorber, chemical intermediate
12.8	β -eudesmol	473-15-4	t.i.	natural compound
12.8	triallylisocyanurate	1025-15-6	t.i.	plastic
12.9	2,6,10-trimethyl-1,5,9-undecatriene	62951-96-6	t.i.	-
12.9	5,9-dimethyl-2- (1-methylethyl) cyclodecane-1,4-dione	38230-97-6	t.i.	-
12.9	3-methylideneundecane	71138-64-2	t.i.	chemical intermediate, natural compound
12.9	globulol	51371-47-2	t.i.	natural compound
12.9	a-bisabolol	515-69-5	t.i.	natural compound, cosmetics
13	tetradecanol	343217-72-1	t.i.	-
13	p-toluenesulfonamide	70-55-3	t.i.	fungicide, coatings, chemical intermediate
13	4-heptadecanone	53685-77-1	t.i.	chemical intermediate
13	5-methoxytryptamine	608-07-1	t.i.	chemical intermediate, hypnotic and sedative enhancer
13	8-heptadecene	16369-12-3	t.i.	natural compound, cosmetics
13	diethyl phthalate	84-66-2	c.i.	plasticizer
13	desethylatrazine	6190-65-4	c.i.	degradation product of herbicide atrazine
13.1	ethyl 4-(4-methoxyphenyl)-2,4-dioxobutanoate	35322-20-4	t.i.	-
13.1	beta-methyl ionone	127-43-5	t.i.	food additive
13.1	desethylterbuthylazine	30125-63-4	c.i.	degradation product of herbicide terbuthylazine
13.2	isopropyl laurate	10233-13-3	t.i.	-
13.2	gamma-dodecalactone	2305-05-7	t.i.	flavors, fragrances
13.2	2-pentadecanol	1653-34-5	t.i.	natural compound, cosmetics
13.2	methylphenylchloridazon	17254-80-7	t.i.	degradation product of herbicide chloridazon
13.3	2-pentadecanone	2345-28-0	t.i.	flavors, fragrances
13.3	heptadecane	629-78-7	t.i.	petroleum products, natural compound
13.3	3,3,6,8-tetramethyl-2,4-dihydronaphthalen-1-one	5409-55-2	t.i.	decomposition of oil
13.3	2-ethylhexyl benzoate	5444-75-7	t.i.	solvent, cosmetics
13.4	octahydro-4,8,8,9-tetramethyl-1,4-methanoazulen-7 (1H) -one	18319-28-3	t.i.	-

13.4	3-methyl-3-heptanol	5582-82-1	t.i.	decomposition of organic materials
13.5	E)-4-(3-hydroxy-1,5,5-trimethyl-7-oxabicyclo[4.1.0]heptan-6-yl)but-3-en-2-one	38274-01-0	t.i.	-
13.5	hexadecanal	629-80-1	t.i.	natural compound, cosmetics
13.6	2- (N-dimethyl-thiocarbamoylthio) -cyclopentanone	23839-30-7	t.i.	-
13.6	3,5-di-tert-butylcatechol	1020-31-1	t.i.	-
13.6	4-hydroxy-3,5-di-tert-butyl-2,4-cyclohexadien-1-one	54965-43-4	t.i.	-
13.8	N-propylbenzoate	2315-68-6	t.i.	cosmetics, flavors, fragrances
13.9	simazine	122-34-9	c.i.	herbicide
14	1-tridecanol	112-70-9	t.i.	chemical intermediate
14	2-dodecenal	4826-62-4	t.i.	natural compound
14	2,6-dichlorobenzamide	2008-58-4	c.i.	degradation product of herbicide 2,6-dichlorobenzonitrile
14.1	4,4-diphenyl-2-pentyne	54372-84-8	t.i.	-
14.1	7a-methyl-3-methylidene-4,5,6,7-tetrahydro-3aH-benzofuran-2-one	67498-53-7	t.i.	-
14.1	octahydro-4a (2H) -oxygenylmethanol	99992-19-5	t.i.	-
14.1	2,5-di-tert-amylhydroquinone	79-74-3	t.i.	antioxidant, gum supplement
14.1	dichloro[1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl]phosphine	74630-16-3	t.i.	pharmaceutical intermediate
14.1	atrazine	1912-24-9	c.i.	herbicide
14.1	dodecanamide	1120-16-7	t.i.	cosmetics, plastic
14.2	3,5-di-tert-butyl-4-hydroxybenzaldehyde	1620-98-0	t.i.	pharmaceutical intermediate
14.2	propazine	139-40-2	c.i.	herbicide
14.2	(Z)-pentatriacont-17-ene	6971-40-0	t.i.	cosmetics
14.2	alpha-copaene-11-ol	41370-56-3	t.i.	natural compound
14.2	myristic acid	544-63-8	t.i.	natural compound
14.3	4-[(4-amino-m-tolyl)amino]phenol	6219-89-2	t.i.	-
14.3	octyl octanoate	2306-88-9	t.i.	flavors, fragrances
14.3	2-geranylphenol	10232-02-7	t.i.	natural compound
14.4	(4-butyl-cyclohex-1-enyl)-benzonitrile	72114-68-2	t.i.	-
14.4	2-nonadecanone	629-66-3	t.i.	natural compound
14.5	terbutylazine	5915-41-3	c.i.	herbicide
14.5	triallyl cyanurate	101-37-1	t.i.	chemical intermediate, plastic
14.6	isopropyl 2-butenolate	18060-77-0	t.i.	natural compound
14.6	N-butylbenzenesulphonamide	3622-84-2	c.i.	plasticizer, chemical intermediate, chlorobenzene metabolite
14.6	tris(2-chloro-1-methylethyl) phosphate	13674-84-5	t.i.	plastic
14.7	1,4,7,10,13,16-hexaoxacyclooctadecane	17455-13-9	t.i.	-
14.8	octahydroacridine	1658-08-8	t.i.	pyrolysis reactions
15	8,9b-dimethyl-4a,9b-dihydrodibenzo[b,d]furan-3(4H)-one	546-24-7	t.i.	-
15.1	2-azacyclotridecanone	947-04-6	t.i.	food additive
15.1	benzil	134-81-6	t.i.	chemical intermediate
15.2	1H-indole-2,3-dione	91-56-5	t.i.	colors, chemical intermediate
15.2	(4-ethylphenyl)-phenylmethanone	18220-90-1	t.i.	chemical intermediate
15.2	isopropyl myristate	110-27-0	t.i.	cosmetics, textile additive
15.2	phytol	150-86-7	t.i.	natural compound
15.3	hexaethylene glycol dimethyl ether	1072-40-8	t.i.	plastic, solvent
15.4	3,7,11,15-tetramethyl-2-hexadecen-1-ol	102608-53-7	t.i.	natural compound
15.5	1,4,7,10,13,16,19-heptaoxacycloheneicosan-2-one	83410-52-0	t.i.	-
15.5	corymbolone	97094-19-4	t.i.	-
15.5	1-methoxy-2-phenoxybenzene	1695-04-1	t.i.	natural compound
15.6	ethylene glycol dimethacrylate	97-90-5	t.i.	polymers

15.7	hexadecennitrile	88592-11-4	t.i.	-
15.7	9E-hexadecen-1-ol	64437-47-4	t.i.	insect pheromone
15.7	benzene-1,4-dicarboxaldehyde	623-27-8	t.i.	chemical intermediate
15.7	hexahydrofarnesyl acetone	502-69-2	t.i.	natural insecticide
15.7	diisobutyl phthalate	84-69-5	t.i.	plasticizer
15.7	caffeine	58-08-2	c.i.	urban waste water
15.8	2,3,3-trimethyl-1-thia-3-silacyclohexane,	88820-74-0	t.i.	-
15.8	tetraethylene glycol dimethacrylate	109-17-1	t.i.	plastic
15.8	desaminometribuzin	35045-02-4	t.i.	the degradation product of herbicide metribuzin
15.8	triethylene glycol dimethacrylate	109-16-0	t.i.	dental materials, contact lenses
15.9	nonadec-9-ene	31035-07-1	t.i.	-
15.9	pentadecanoic acid	1002-84-2	t.i.	-
15.9	antipyrine	60-80-0	t.i.	analgesic
15.9	2,4-dimethoxyphenyl isothiocyanate	33904-03-9	t.i.	chemical intermediate
16	1-nonadecene	18435-45-5	t.i.	petroleum products
16	tetra(ethylene glycol) bis(2-ethylhexanoate)	18268-70-7	t.i.	plasticizer
16	hexadecanenitrile	629-79-8	t.i.	pyrolysis product
16	mebicar	10095-06-4	t.i.	pharmaceuticals
16	trans-1-methoxy-3-trimethylsiloxy-1,3-butadiene 95	38913-02-9	t.i.	
16.1	methyl 9(E)-hexadecenoate	10030-74-7	t.i.	natural compound
16.2	3-benzylpentane-2,4-dione	1134-87-8	t.i.	-
16.3	metribuzin	21087-64-9	c.i.	herbicide
16.4	2-heptadecanone	2922-51-2	t.i.	natural compound
16.4	dechlorometazachlor	-	t.i.	degradation product of herbicide metazachlor
16.5	4,5,9,10-dehydroisolongifolene	156747-45-4	t.i.	natural compound
16.5	7,9-di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene- 2,8-dione	82304-66-3	t.i.	plastic
16.6	3,4-dimethylbenzophenone	2571-39-3	t.i.	chemical intermediate
16.6	palmitoleic acid methyl ester	1120-25-8	t.i.	natural compound
16.7	prometryn	7287-19-6	c.i.	herbicide
16.8	methyl palmitate	112-39-0	t.i.	chemical intermediate
17	N- (1,4-dihydro-2,2-dimethyl-4-oxo-3 (2H) - quinazoline) -acetamide	309732-49-8	t.i.	-
17	(Z)-11-hexadecenoic acid	2416-20-8	t.i.	natural compound
17	pentaethylene glycol monomethyl ether	23778-52-1	t.i.	solvent, plastic additive
17.1	N-acetyltyramine	1202-66-0	t.i.	pharmaceuticals
17.2	1-hexadecanol	36653-82-4	t.i.	emulsifier, cosmetics
17.2	5-methoxygramine	16620-52-3	t.i.	pharmaceutical intermediate
17.2	terbutryn	886-50-0	c.i.	herbicide
17.3	1,2,2-trimethylbutyl)cyclohexane	61142-21-0	t.i.	-
17.3	dibutyl phthalate	84-74-2	c.i.	plasticizer
17.4	palmitic acid	57-10-3	t.i.	emulsions, polymer coatings, food
17.4	9-hexadecenoic acid	2091-29-4	t.i.	natural compound, oils
17.4	propyphenazone	479-92-5	c.i.	pharmaceuticals
17.5	bromacil	314-40-9	t.i.	herbicide
17.7	metalaxyl	57837-19-1	c.i.	herbicide
17.7	metolachlor	51218-45-2	c.i.	herbicide
17.8	lidocaine	137-58-6	t.i.	pharmaceuticals
18.2	1,3,5-tri-tert-butylbenzene	1460-02-2	t.i.	plastic
18.4	1,2-bis-(2'-hydroxyphenyl)ethane	29338-20-3	t.i.	-
18.5	(4-isopropyl-phenyl)-phenyl-methanone	18864-76-1	t.i.	-
18.6	4-hydroxy-5,6-epoxy beta ionone	900108-78-1	t.i.	-
18.6	8-propoxycedrane	19870-75-8	t.i.	tobacco smoke

18.6	aminophenazone	58-15-1	t.i.	pharmaceuticals
18.7	2,2,4,4,6,8,8-heptamethylnonane	4390-04-9	t.i.	decomposition of oil
18.8	bufencarb		t.i.	insecticide
18.8	5-phenyl-1,3-thiazole-2,4-diamine	490-55-1	t.i.	pharmaceuticals
19	4-O-acetyl-3-methoxy-oylene-1,4-diol	116461-66-6	t.i.	-
19	2,5-di-ter-butyl-1,4-benzoquinon	2460-77-7	t.i.	pharmaceutical intermediate
19.1	metazachlor	67129-08-2	c.i.	herbicide
19.1	carbamazepine-M (formyl acridine)	-	t.i.	metabolite of carbamazepine
19.2	arachidonic acid	506-32-1	t.i.	natural compound
19.6	4-(hexyloxy)-1-butanol	4541-13-3	t.i.	-
19.6	cyclooctasulfur	10544-50-0	t.i.	oil, tires, sulfate reduction
19.7	1, 13-tridecanediol diacetate	42236-70-4	t.i.	-
19.7	methyl oleate	112-62-9	t.i.	natural compound
19.8	3-methyl-1-penten-3-ol	918-85-4	t.i.	-
19.9	stearoyl chloride	112-76-5	t.i.	chemical intermediate
20	phenobarbital	50-06-6	t.i.	pharmaceuticals
20.3	bis(2-ethylhexyl) phthalate	131-18-0	t.i.	plasticizer
20.6	cedrol	77-53-2	t.i.	flavors, fragrances
20.6	gibberellin A9	427-77-0	t.i.	natural fungicide
20.9	methyl stearate	112-61-8	t.i.	chemical intermediate, cosmetics
21.3	2,5-bis(trifluoromethyl)bromobenzene	15674-93-8	t.i.	-
21.3	heptan-4-ol	7316-84-9	t.i.	-
21.3	oleic acid	112-80-1	t.i.	general purpose chemical, natural compound
21.3	hexahydro-1H-pyrrolizine-3,5-dione	18356-28-0	t.i.	pharmaceuticals
21.5	dihydrophytol	645-72-7	t.i.	natural compound
21.5	octadec-1-ene	112-88-9	t.i.	solvent, chemical intermediate
21.6	stearic acid	57-11-4	t.i.	chemical intermediate, cosmetics, pharmacy
21.8	methyl 3-(diphenylphosphanyl)propanoate	76734-29-7	t.i.	-
21.8	bisphenol A	80-05-7	t.i.	plastic additive, antioxidant
21.9	hexadecanamide	629-54-9	t.i.	plastic additive
22	tributyl citrate	77-94-1	t.i.	plasticizer, surfactant
22.1	butyl hexadecanoate	111-06-8	t.i.	cosmetics, food additive
22.3	mephenoxalone	70-07-5	t.i.	medicine
22.4	11(Z)-octadecenoic acid	506-17-2	t.i.	natural compound
22.5	triethylene glycol bis(2-ethylhexanoate)	94-28-0	t.i.	plasticizer
22.6	octaethylene glycol	5117-19-1	t.i.	food additive, plasticizer
22.9	3,6,9,12,15-pentaoxonadecan-1-ol	1786-94-3	t.i.	chemical intermediate, solvent, addition to polymers
22.9	1-heptadecanol	822-20-8	t.i.	natural compound
23.1	1,8-diazacyclotetradecane-2,7-dione	4266-66-4	t.i.	-
23.3	cis-9-octadecen-1-ol	143-28-2	t.i.	cosmetics, natural compound
23.5	tributyl o-acetylcitrate	77-90-7	t.i.	plasticizer, flavours
23.6	1,8-diazacyclotetradecane-2,9-dione	5776-79-4	t.i.	-
24.7	metolachlor-M m/z 162,282	-	t.i.	degradation product of herbicide metolachlor
24.8	nifedipine metabolite artifact	99982-48-6	t.i.	thermal decay of the metabolite of nifedipine
25.3	tris(1,3-dichloro-2-propyl) phosphate	13674-87-8	t.i.	plasticizer, a flame retardant in plastic
25.4	2-[2-[2-[2-(2-methoxy methoxy)metoxi]metoxi]metoxi]etanol	*NIST 352040	t.i.	lubricants, plasticizer, cosmetics
25.6	methyl ester-11,14-eicosadienoic acid	2463-02-7	t.i.	natural compound
25.7	linoleic acid	60-33-3	t.i.	emulsions, polymer coatings, food
25.7	carbamazepine	298-46-4	c.i.	pharmaceuticals
25.7	4-methylaminoantipyrine hydrochloride	519-98-2	t.i.	pharmaceuticals
25.9	N-lauroyl-DL-homoserine lactone	18627-38-8	t.i.	-
26.4	tebuconazole	107534-96-3	t.i.	fungicide

26.7	butyl stearate	123-95-5	t.i.	flavor, additives
27	tris(2-butoxyethyl) phosphate	78-51-3	t.i.	plasticizer
27.1	bis(2-ethylhexyl) adipate	103-23-1	t.i.	cosmetics
27.4	tetrateetracontane	7098-22-8	t.i.	-
27.7	α -curcumene	644-30-4	t.i.	natural compound
27.9	pentadecanal	2765-11-9	t.i.	natural compound
28.8	dodecaethylene glycol	6790-09-6	t.i.	plasticizer
28.9	6-tert-butyl-1,1-dimethyl-2,3-dihydro-1H-inden-4-yl)acetic acid	55591-05-4	t.i.	-
28.9	14-isopropyl-podocarpa-8,11,13-triene-7,13-diol	24338-19-0	t.i.	-
29	4-hydroxybutyl acrylate	55134-10-6	t.i.	-
29.3	dibutylamin	111-92-2	t.i.	-
29.5	8-hexylpentadecane	13475-75-7	t.i.	natural compound
29.8	diisooctyl phthalate	27554-26-3	t.i.	plasticizer
29.8	mono-ethylhexyl ester	4376-20-9	t.i.	plasticizer
29.9	bis(2-ethylhexyl) phthalate	117-81-7	c.i.	plasticizer
30.9	triphenylphosphine oxide	791-28-6	t.i.	pharmaceutical intermediate
31.1	tetradecyl dodecanoate	22412-97-1	t.i.	cosmetics
31.2	nandrolone	434-22-0	t.i.	pharmaceuticals
31.4	di-n-octyl phthalate	117-84-0	t.i.	plasticizer
32.6	16-heptadecenal	900144-57-9	t.i.	-
33.3	2,4-bis(α,α -dimethylbenzyl)phenol	2772-45-4	t.i.	antioxidant, plastic additive
34.4	bis(2-ethylhexyl) isophthalate	137-89-3	t.i.	plastic additive
35.2	cis-9,10-octadecenoamide	301-02-0	t.i.	additive to reduce wear and tear on polyethylene expansion
35.5	celecoxib	169590-42-5	t.i.	pharmaceuticals
35.7	octacosane	630-02-4	t.i.	-
35.8	octadecanamide	124-26-5	t.i.	chemical intermediate, corrosion inhibitor
36.1	squalene	7683-64-9	t.i.	natural compound
36.3	16 α -tert.-butyl- Δ 5-androstenol-(3 β)-on-(17)-halbmethanolat	55162-58-8	t.i.	steroid
36.5	27-nor-25-ketocholesterol	7494-34-0	t.i.	intermediat
38.5	2-methyloctadecane	1560-88-9	t.i.	petroleum products
38.9	cholesta-3,5-diene	747-90-0	t.i.	steroid, natural compound
39.1	n-octanoic anhydride	623-66-5	t.i.	-
39.2	praziquantel	55268-74-1	t.i.	pharmaceuticals
39.3	1-heptacosanol	2004-39-9	t.i.	natural compound
41.3	1,4-butanediol diglycidyl ether	2425-79-8	t.i.	chemical intermediate
41.8	cholesterol	57-88-5	t.i.	hormone, slurry, septic tanks, sewage
41.9	loratadine	79794-75-5	t.i.	pharmaceuticals
44.3	4-cholesten-3-one	601-57-0	t.i.	steroid, slurry, septic tanks, sewage
45.2	stigmasterol	83-48-7	t.i.	steroid, slurry, septic tanks, sewage
45.3	gamma-sitosterol	83-47-6	t.i.	steroid
45.8	dilaurin	17598-94-6	t.i.	natural compound, food
47.5	palmityl palmitate	540-10-3	t.i.	natural compound
48.4	olean-12-en-3-one	638-97-1	t.i.	-
49.2	beta-amyirin	559-70-6	t.i.	natural triterpene compound
49.8	2,6,10,15,19,23-hexamethyl-tetracos-2,10,14,18,22-pentaene-6,7-diol	*NIST194707	t.i.	natural compound