

Substance					Application			Statistics
Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
1,1-Oxybis(2,4,5-tribromobenzene)	BDE-153	C12H4Br6O	643.58	68631-49-1	Industrial Agents	Flame retardant	Parent	11
1,2,3,5-tetrabromo-4-(2,4,5-tribromophenoxy)benzene	BDE-183	C12H3Br7O	722.48	207122-16-5	Industrial Agents	Flame retardant	Parent	11
1,2,3-Trichlorbenzene		C6H3Cl3	181.45	87-61-6	Industrial Agents	Production of Pharmaceuticals, Pesticides, Paint, Solving Agent	Intermediate	2
1,2,4-Trichlorbenzene		C6H3Cl3	181.45	120-82-1	Industrial Agents	Production of Pharmaceuticals, Pesticides, Paint, Solving Agent	Intermediate	4
1,3,5-tribromo-2-(2,4,5-tribromophenoxy)benzene	BDE-154	C12H4Br6O	643.58	207122-15-4	Industrial Agents	Flame retardant	Parent	11
1,3,5-Tribromobenzene	BDE-100	C12H5Br5O	564.69	626-39-1	Industrial Agents	Flame retardant	Parent	11
1,3,5-Trichlorbenzene		C6H3Cl3	181.45	108-70-3	Industrial Agents	Production of Pharmaceuticals, Pesticides, Paint, Solving Agent	Intermediate	4
1,5-Naphthalenesulfonic acid		C10H8O3S	208.23	84-89-9	Industrial Agents	Detergents	Parent	1
1,7-Naphthalenesulfonic acid		C10H8O3S	208.23		Industrial Agents	Detergents	Parent	1
10,11-Dihydro-10,11-Epoxycarbamazepine	Carbamazepine-10,11-epoxide	C15H12N2O2	252.27	36507-30-9	Pharmaceutics	Anticonvulsant	Transformation Product	29
16a-Hydroxyestrone		C18H22O3	286.37	15270-34-5	Pharmaceutics	Estrogen	Transformation Product	11
17a-Ethinylestradiol		C20H24O2	296.40	57-63-6	Pharmaceutics	Estrogen	Parent	11
17-alpha-Estradiol		C18H24O2	272.38	57-91-0	Pharmaceutics	Estrogen	Parent	8
17-alpha-Ethinylestradiol		C20H24O2	296.40	57-63-6	Pharmaceutics	Estrogen	Parent	77
17-beta-Estradiol		C18H24O2	272.18	50-28-2	Pharmaceutics	Estrogen	Parent	76
1H-Benzotriazole		C6H5N3	119.12	95-14-7	Industrial Agents	Anticorrosive agent	Parent	59
2,2',4,4',5-Pentabromodiphenyl ether	BDE-99	C12H5Br5O	564.69	32534-81-9	Industrial Agents	Flame retardant	Parent	11
2,4,5-Trichlorophenoxyacetic acid	2,4,5-T	C8H5Cl3O3	255.48	93-76-5	Pesticide	Herbicide	Parent	14
2,4,7,9-Tetramethyl-5-decin-4,7-diol	TMDD	C14H26O2	226.36	126-86-3	Industrial Agents	Tenside	Parent	12
2,4-Dibromo-1-(4-bromophenoxy)benzene	BDE-28	C12H7Br3O	406.90	41318-75-6	Industrial Agents	Flame retardant	Parent	11
2,4-Dichlorophenoxyacetic acid	2,4-D	C6H4N2O5	184.11	94-75-7	Pesticide	Herbicide, Fungicide	Parent	33
2,4-Dinitrophenol	2,4-DNP	C6H4N2O5	184.01	51-28-5	Pesticide	Herbicide, Fungicide	Parent	19
2,7-Naphthalenesulfonic acid		C10H8O3S	208.23	120-18-3	Industrial Agents	Petro Industry	Parent	1
2-Bromobiphenyl		C12H9Br	233.10	2052-07-5	Industrial Agents	Flame retardant	Parent	11
2-Ethyl-Hexyl-4-Trimethoxycinnamate	2-EHMC	C18H26O3	290.40	5466-77-3	Personal Care Product	Cosmetics	Parent	9
2-Ethylhexyldiphenylphosphate	EHDPP	C20H27O4P	362.40	1241-94-7	Industrial Agents	Flame retardant	Parent	14

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Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
2-Hydroxy Ibuprofen		C13H18O3	222.13	51146-55-5	Pharmaceutics	Analgesics	Transformation Product	2
2methyl-4-chlorophenoxyacetic acid	MCPA	C9H9ClO3	200.62	94-74-6	Pesticide	Pesticide	Parent	14
3,4-Methylenedioxy-N-methylamphetamin	MDMA	C11H15NO2	193.25	42542-10-9	Pharmaceutics	Psychoactive Substance	Parent	3
4-Acetaminoantipyrine		C13H15N3O2	245.12	83-15-8	Pharmaceutics	Analgesics	Transformation Product	15
4-Aminoantipyrine		C11H13N3O	203.24	83-07-8	Pharmaceutics	Analgesics	Transformation Product	12
4-Epitetracycline		C22H24N2O8	444.44	23313-80-6	Pharmaceutics	Antibiotics	Transformation Product	3
4-Formylaminoantipyrine		C12H13N3O2	231.25	1672-58-8	Pharmaceutics	Analgesics	Transformation Product	1
4-Hydroxydiclofenac		C14H11Cl2NO3	312.15	64118-84-9	Pharmaceutics	Analgesics	Transformation Product	4
4-Hydroxyomeprazole		C16H17N3S	331.10	103876-98-8	Pharmaceutics	proton pump inhibitors	Transformation Product	5
4-Methylaminoantipyrine		C12H15N3O	217.27	519-98-2	Pharmaceutics	Analgesics	Transformation Product	4
4-Methylbenzylidene camphor	4-MBC	C18H22O	254.37	36861-47-9	Personal Care Product	Cosmetics	Parent	6
4-N-Nonylphenol		C15H24O	220.18	104-40-5	Industrial Agents	Detergents	Intermediate	11
4-N-Octylphenol		C14H22O	206.32	140-66-9	Industrial Agents	Production of resin, paint etc.	Intermediate	8
5-Methyl-1H-benzotriazole		C7H7N3	133.15	136-85-6	Industrial Agents	Complexing Agent	Parent	13
6-Acetylmorphine		C19H21NO4	327.37	2784-73-8	Pharmaceutics	Morphine derivates	Transformation Product	3
6-O-Desmethylnaproxen		C13H12O3	216.23	52079-10-4	Pharmaceutics	Anti-inflammatory drug	Transformation Product	2
7-Aminonitrazepam		C15H13N3O	251.28	4928-02-3	Pharmaceutics	Anticonvulsant	Transformation Product	2
Acebutolol		C18H28N2O4	336.43	37517-30-9	Pharmaceutics	Beta blockers	Parent	12
Acesulfame K		C4H4KNO4S	201.24	55589-62-3	Food Additives	Sweetener	Parent	25
Acetoaminoantipyrine		C13H15N3O2	245.28	83-15-8	Pharmaceutics	Analgesics	Transformation Product	9
Acetylsalicylic acid		C9H8O4	180.16	50-78-2	Pharmaceutics	Analgesics	Parent	17
Acridone		C13H9NO	195.22	578-95-0	Pharmaceutics	Psychiatric medication	Parent	1
Alachlor		C14H20ClNO2	269.77	15972-60-8	Pesticide	Herbicide	Parent	2
Albendazole		C12H15N3O2S	265.33	54965-21-8	Pharmaceutics	Anthelmintics	Parent	1
Alfuzosin		C19H27N5O4	389.45	81403-80-7	Pharmaceutics	Alpha blockers	Parent	14
Alprazolam		C17H13ClN4	308.77	28981-97-7	Pharmaceutics	Antidepressant	Parent	9

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Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Amidotrizoic acid		C11H9I3N2O4	613.91	117-96-4	Pharmaceutics	Radiocontrast agents	Parent	12
Amitriptyline		C20H23N	277.40	50-48-6	Pharmaceutics	Antidepressant	Parent	22
Amlodipine		C20H25ClN2O5	408.88	88150-42-9	Pharmaceutics	Calcium Channel Blocker	Parent	2
Amoxicillin		C16H19N3O5S	365.40	26787-78-0	Pharmaceutics	Antibiotics	Parent	28
Amphetamine		C9H13N	135.21	300-62-9	Pharmaceutics	Sympathomimetic drugs	Parent	3
Ampicillin		C16H19N3O4S	349.41	69-53-4	Pharmaceutics	Antibiotics	Parent	3
Androstenedione		C19H26O2	286.41	5982-99-0	Pharmaceutics	Steroid	Parent	2
Androsterone		C19H30O2	290.44	63-05-8	Pharmaceutics	Steroid	Parent	2
Anhydroerythromycin		C37H65NO12	715.91	23893-13-2	Pharmaceutics	Antibiotics	Transformation Product	2
Anthracene		C14H10	178.23	1719-06-8	Industrial Agents	Production of Paint, Pesticides	Intermediate	2
Antipyrine		C11H12N2O	188.10	519-98-2	Pharmaceutics	Analgesics	Parent	1
Atenolol		C14H22N2O3	266.34	29122-68-7	Pharmaceutics	Beta blockers	Parent	224
Atorvastatin		C33H35FN2O5	558.64	134523-00-5	Pharmaceutics	Lipid-lowering drugs	Parent	44
Atrazine		C8H14ClN5	215.68	1912-24-9	Pesticide	Herbicide	Parent	61
Atrazine-desethyl		C6H10ClN5	187.63	6190-65-4	Pesticide	Herbicide	Transformation Product	28
Azithromycin		C38H72N2O12	748.98	83905-01-5	Pharmaceutics	Antibiotics	Parent	92
Bentazone		C10H12N2O3S	240.28	25057-89-0	Pesticide	Herbicide	Parent	34
Benzofluoranthene		C20H12	252.31	205-82-3	Industrial Agents	Petro Industry	Intermediate	8
Benzoperylene		C24H14	302.37	191-85-5	Industrial Agents	Production of Paint	Intermediate	2
Benzophenone		C13H10O	182.22	119-61-9	Industrial Agents	Photo inhibitor	Parent	3
Benzopyrene		C20H12	252.32	50-32-8	Industrial Agents	Petro Industry	Intermediate	5
Benzothiazole		C7H5NS	135.19	95-16-9	Industrial Agents	Rubber Industry	Intermediate	14
Benzoyllecgonine		C16H19NO4	289.33	519-09-5	Pharmaceutics	Analgesics	Parent	7
Benzylparaben		C14H12O3	228.24	94-18-8	Industrial Agents	Preservative	Intermediate	2
Benzylpenicillin		C16H18N2O4S	334.39	61-33-6	Pharmaceutics	Antibiotics	Parent	3
Betaxolol		C18H29NO3	307.43	63659-18-7	Pharmaceutics	Beta blockers	Parent	11
Bezafibrate		C19H20ClNO4	361.82	41859-67-0	Pharmaceutics	Lipid-lowering drugs	Parent	287
Biperiden		C21H29NO	311.46	514-65-8	Pharmaceutics	Anticholinergics	Parent	7
bis(3,4-dibromophenyl) ether	pBDE-77	C12H6Br4O	485.79	93703-48-1	Industrial Agents	Flame retardant	Parent	5
Bisoprolol		C18H31NO4	325.44	66722-44-9	Pharmaceutics	Beta blockers	Parent	42
Bisphenol A		C15H16O2	228.29	80-05-7	Industrial Agents	Production of plastics	Parent	72

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Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Bromazepam		C14H10BrN3O	316.15	1812-30-2	Pharmaceutics	Anxiolytics	Parent	17
Budesonide		C25H34O6	430.53	51333-22-3	Pharmaceutics	Glucocorticoids	Parent	9
Bupropion		C13H18CINO	239.74	34841-39-9	Pharmaceutics	Antidepressant	Parent	11
Butalbital		C11H16N2O3	224.26	77-26-9	Pharmaceutics	Analgesics	Parent	4
Butylhydroxytoluol	BHT	C15H24O	220.35	128-37-0	Personal Care Product	Cosmetics, Packaging Material, Food additive	Parent	10
Caffeine		C8H10N4O2	194.19	58-08-2	Food Additives	Stimulant	Parent	71
Carazolol		C18H22N2O2	298.38	57775-29-8	Pharmaceutics	Beta blockers	Parent	4
Carbamazepine		C15H12N2O2	236.27	298-46-4	Pharmaceutics	Antiepileptic drugs	Parent	508
Carbamazepine-2OH				68011-66-5	Pharmaceutics	Antiepileptic drugs	Transformation Product	6
Carbamazepine-3OH					Pharmaceutics	Antiepileptic drugs	Transformation Product	4
Carbaryl		C12H11NO2	201.22	63-25-2	Pesticide	Insecticide	Parent	13
Carvedilol		C24H26N2O4	406.47	72956-09-3	Pharmaceutics	Beta blockers	Parent	1
Cashmeran		C14H22O	206.32	33704-61-9	Personal Care Product	Fragrance	Parent	8
Cashmerane	DPMI	C14H22O	206.32	33704-61-9	Personal Care Product	Cosmetics	Parent	12
Cefalexin		C16H17N3O4S	347.39	15686-71-2	Pharmaceutics	Antibiotics	Parent	3
Cefapirin		C17H17N3O6S2	423.46	21593-23-7	Pharmaceutics	Antibiotics	Parent	3
Cefazolin		C14H14N8O4S3	454.51	25953-19-9	Pharmaceutics	Antibiotics	Parent	3
Cefotaxime		C16H17N5O7S2	455.47	63527-52-6	Pharmaceutics	Antibiotics	Parent	6
Ceftiofur		C19H17N5O7S3	523.56	80370-57-6	Pharmaceutics	Antibiotics	Parent	3
Celestolid	ADBI	C17H24O	244.37	13171-00-1	Personal Care Product	Cosmetics, Musk Fragrances	Parent	12
Celestolide		C17H24O	244.37	13171-00-1	Personal Care Product	Polycyclic musks	Parent	8
Cetirizine		C21H25CIN2O3	388.89	83881-51-0	Pharmaceutics	Antihistamine	Parent	10
Chloramphenicol		C11H12Cl2N2O5	323.13	56-75-7	Pharmaceutics	Antibiotics	Parent	16
Chlordiazepoxide		C16H14CIN3O	299.76	58-25-3	Pharmaceutics	Hypnotics	Parent	8
Chlorfenvin		C12H8Cl2O3S	303.16	80-33-1	Pharmaceutics	Antiparasitics	Parent	1
Chlorfenvinphos A		C12H14Cl3O4P	359.57	470-90-6	Pharmaceutics	Antiparasitics	Parent	3
Chlorfenvinphos B		C12H14Cl3O4P	359.57	470-90-6	Pharmaceutics	Antiparasitics	Parent	2
Chlorotoluron		C10H13CIN2O	212.68	15545-48-9	Pesticide	Herbicide	Parent	13
Chlorpyrifos-ethyl		C0H11Cl3NO3PS	350.58	2921-88-2	Personal Care Product	Insect Repellent	Parent	10
Chlortetracycline		C22H23CIN2O8	478.88	57-62-5	Pharmaceutics	Antibiotics	Parent	21

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Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Cilazapril		C22H31N3O5	417.50	88768-40-5	Pharmaceutics	ACE inhibitor	Parent	2
Cimetidine		C10H16N6S	252339.00	51481-61-9	Pharmaceutics	Antacids	Parent	28
Cinoxacin		C12H10N2O5	262.22	28657-80-9	Pharmaceutics	Antibiotics	Parent	3
Ciprofloxacin		C17H18FN3O3	331.34	85721-33-1	Pharmaceutics	Antibiotics	Parent	119
Cis-Chlorfenvinphos		C12H14Cl3O4P	359.57	470-90-6	Pharmaceutics	Antiparasitics	Parent	3
Citalopram		C <sub>20</sub> H <sub>21</sub> FN <sub>2</sub> O	324.39	59729-33-8	Pharmaceutics	Antidepressant	Parent	48
Citalopram HBr		C20H22BrFN2O	405.30	59729-32-7	Pharmaceutics	Antidepressant	Parent	1
Clarithromycin		C38H69NO13	747.95	81103-11-9	Pharmaceutics	Antibiotics	Parent	145
Clenbuterol		C12H18Cl2N2O	277.19	37148-27-9	Pharmaceutics	Anti-asthmatics	Parent	11
Clindamycin		C18H33ClN2O5S	424.98	18323-44-9	Pharmaceutics	Antibiotics	Parent	14
Clofibric acid		C10H11ClO3	214.65	882-09-7	Pharmaceutics	Lipid-lowering drugs	Transformation Product	127
Clomipramine		C19H23ClN2	314.85	303-49-1	Pharmaceutics	Antidepressant	Parent	19
Clonazepam		C15H10ClN3O3	315.71	1622-61-3	Pharmaceutics	Anticonvulsant	Parent	2
Clopidogrel		C16H16ClNO2S	321.82	113665-84-2	Pharmaceutics	Antiplatelet agent	Parent	4
Clotrimazole		C22H17ClN2	344.84	23593-75-1	Pharmaceutics	Antifungal medication	Parent	11
Cloxacillin		C19H18ClN3O5S	435.88	61-72-3	Pharmaceutics	Antibiotics	Parent	2
Cocaethylene		C18H23NO4	317.38	529-38-4	Other	Psychoactive Substance	Transformation Product	3
Cocaine		C17H21NO4	303.36	53-21-4	Other	Psychoactive Substance	Parent	3
Codeine		C18H21NO3	299.36	76-57-3	Pharmaceutics	Morphine derivates	Parent	47
Cortisol		C21H30O5	362.46	50-23-7	Pharmaceutics	Glucocorticoids	Parent	1
Cortisone		C21H28O5	360.44	53-06-5	Pharmaceutics	Glucocorticoids	Parent	1
Cotinine		C10H12N2O	176.22	486-56-6	Personal Care Product	Nicotine metabolite	Transformation Product	1
Cyanazine		C9H13ClN6	240.69	21725-46-2	Pesticide	Pesticide	Parent	2
Cyclamate		C6H12NNaO3S	201.22	139-05-9	Food Additives	Sweetener	Parent	11
Cyclophosphamide		C7H15Cl2N2O2P	261.09	50-18-0	Pharmaceutics	Chemotherapeutic agents	Parent	15
Danofloxacin		C19H20FN3O3	357.38	112398-08-0	Pharmaceutics	Antibiotics	Parent	10
Decamethylcyclopentasiloxane	D5	C10H30O5Si5	370.77	541-02-6	Personal Care Product	Cosmetics, Washing Agent	Parent	12
Decamethyltetrasiloxane	MD2M	C10H30O3Si4	310.69	141-62-8	Personal Care Product	Cosmetics	Parent	12
Deethylatrazine		C6H10ClN5	187.63	6190-65-4	Pesticide	Pesticide	Transformation Product	1

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Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Deethylcyanazine				21725-40-6	Pesticide	Pesticide	Transformation Product	2
Dehydrato-Erythromycin					Pharmaceutics	Antibiotics	Transformation Product	11
Deisopropylatrazine		C5H8CIN5	173.60	1007-28-9	Pesticide	Pesticide	Transformation Product	1
Desethylterbutylazin				30125-63-4	Pesticide	Pesticide	Transformation Product	22
Desvenlafaxine				93413-62-8	Pharmaceutics	Antidepressant	Transformation Product	3
Diatrizoic acid		C11H9I3N2O4	613.91	117-96-4	Pharmaceutics	Radiocontrast agents	Parent	18
Diazepam		C16H13CIN2O	284.74	439-14-5	Pharmaceutics	Psychiatric medication	Parent	89
Diazinon		C12H21N2O3PS	304.35	333-41-5	Pharmaceutics	Insecticides	Parent	42
Dibromobiphenyl		C12H8Br2	312.00	53592-10-2	Industrial Agents	Flame retardant	Parent	11
Dibutylphtalate		C16H22O4	278.34	84-74-2	Industrial Agents	Plasticizer (PVC), Adsorbens	Parent	2
Dichlorprop		C9H8Cl2O3	235.06	120-36-5	Pesticide	Herbicide	Parent	14
Diclofenac		C14H11Cl2NO2	296.15	15307-86-5	Pharmaceutics	Analgesics	Parent	441
Didealkylatrazine		C3H4CIN5	145.55	3397-62-4	Pesticide	Pesticide	Transformation Product	1
Diethylphtalate		C12H14O4	222.24	84-66-2	Industrial Agents	Production of Pesticides, Fragances, Plasticizer	Intermediate	2
Diethylstilbestrol		C18H20O2	268.35	56-53-1	Pharmaceutics	Estrogen	Parent	14
Diltiazem		C22H26N2O4S	414.52	42399-41-7	Pharmaceutics	Antiarrhythmic agents	Parent	23
Dimethyl phtalate		C10H10O4	194.19	131-11-3	Industrial Agents	Plasticizer, Repellent	Parent	4
Dimethylaminophenazone		13H17N3O	231.29	58-15-1	Pharmaceutics	Analgesics	Parent	2
Dinitrophenol		C6H4N2O5	184.11	51-28-5	Industrial Agents	Intermediate in Paint Production, Arms Industry and Pharma Industry	Intermediate	14
Diphenhydramine		C17H21NO	255.36	58-73-1	Pharmaceutics	Antihistamine	Parent	14
Diuron		C9H10Cl2N2O	233.09	330-54-1	Pesticide	Herbicide	Parent	39
Diuron, (3-(3,4-dichlorophenyl)-1,1-dimethylurea)	DCMU	C9H10Cl2N2O	233.09	330-54-1	Pesticide	Herbicide	Parent	13
Dodecamethylcyclohexasiloxane	D6	C12H36O6Si6	444.92	540-97-6	Personal Care Product	Cosmetics, Washing Agent	Parent	12
Doxycycline		C22H26N2O9	462.45	564-25-0	Pharmaceutics	Antibiotics	Parent	21
Enalapril		C20H28N2O5	376.45	75847-73-3	Pharmaceutics	Antihypertensives	Parent	27
Endosulfan II		C9H6Cl6O3S	406.93	115-29-7	Pesticide	Insecticide	Parent	6
Enoxacin		C15H17FN4O3	320.32	74011-58-8	Pharmaceutics	Antibiotics	Parent	17
Enrofloxacin		C19H22FN3O3	359.40	93106-60-6	Pharmaceutics	Antibiotics	Parent	20

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Eprosartan		C23H24N2O4S	424.51	133040-01-4	Pharmaceutics	Antihypertensives	Parent	11
Erythromycin		C37H67NO13	733.93	114-07-8	Pharmaceutics	Antibiotics	Parent	150
Erythromycin-H2O				59319-72-1	Pharmaceutics	Antibiotics	Parent	9
Estradiol		C18H24O2	272.38	50-28-2	Pharmaceutics	Estrogen	Parent	30
Estradiol-17-glucuronide				15087-02-2	Pharmaceutics	Estrogen	Transformation Product	14
Estriol		C18H24O3	288.38	50-27-1	Pharmaceutics	Estrogen	Parent	102
Estriol-16-glucuronide				1852-50-2	Pharmaceutics	Estrogen	Transformation Product	14
Estrone		C18H22O2	270.37	53-16-7	Pharmaceutics	Estrogen	Parent	133
Estrone-3-sulfate		C18H22O5S	350.43	438-67-5	Pharmaceutics	Estrogen	Parent	17
Ethylenediaminetetraacetic acid	EDTA	C10H16N2O8	292.24	60-00-4	Industrial Agents	Complexing Agent	Parent	12
Ethylhexyl methoxycinnamate		C18H26O3	290.40	5466-77-3	Personal Care Product	Cosmetics	Parent	4
Ethylparaben		C9H10O3	166.17	120-47-8	Personal Care Product	Food Additive, Cosmetics	Parent	6
Etofibrate		C18H18ClNO5	363.79	31637-97-5	Pharmaceutics	Lipid-lowering drugs	Parent	12
Etonogestrel		C22H28O2	324.46	54048-10-1	Pharmaceutics	Contraceptiva	Parent	13
Famotidine		C8H15N7O2S3	337.45	76824-35-6	Pharmaceutics	Antihistamine	Parent	43
Fenofibrate		C20H21ClO4	360.83	49562-28-9	Pharmaceutics	Lipid-lowering drugs	Parent	52
Fenofibric acid		C17H15ClO4	318.75	42017-89-0	Pharmaceutics	Lipid-lowering drugs	Transformation Product	25
Fenoprofen		C15H14O3	242.27	31879-05-7	Pharmaceutics	Analgesics	Parent	19
Fentanyl		C22H28N2O	336.47	437-38-7	Pharmaceutics	Analgesics	Parent	1
Fexofenadine		C32H39NO4	501.66	83199-24-0	Pharmaceutics	Antihistamine	Parent	10
Flecainide		C17H20F6N2O3	414.34	54143-55-4	Pharmaceutics	Antiarrhythmic agents	Parent	14
Fluconazole		C13H12F2N6O	306.27	86386-73-4	Pharmaceutics	Antifungal medication	Parent	14
Flumequine		C14H12FNO3	261.25	42835-25-6	Pharmaceutics	Antibiotics	Parent	25
Flunisolide		C24H31FO6	434.50	3385-03-3	Pharmaceutics	Glucocorticoids	Parent	1
Flunixin		C14H11F3N2O2	296.25	38677-85-9	Pharmaceutics	Nonsteroidal Anti-inflammatory drug	Parent	9
Fluocinolone acetonide		C24H30F2O6	452.49	67-73-2	Pharmaceutics	Glucocorticoids	Parent	1
Fluorantene		C16H10	202.26	206-44-0	Industrial Agents	Production of Drugs and Pharmaceutics	Intermediate	2
Fluoxetine		C17H18F3NO	309.33	54910-89-3	Pharmaceutics	Antidepressant	Parent	68
Flupentixol		C23H25F3N2OS	434.52	2709-56-0	Pharmaceutics	Psychiatric medication	Parent	1
Fluvastatin		C24H26FNO4	411.47	93957-54-1	Pharmaceutics	Lipid-lowering drugs	Parent	1

Substance					Application			Statistics
Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Furaltadone		C13H16N4O6	324.29	139-91-3	Pharmaceutics	Antibiotics	Parent	1
Furosemide		C12H11ClN2O5S	330.74	54-31-9	Pharmaceutics	Diuretics	Parent	148
Gabapentin		C9H17NO2	171.24	60142-96-3	Pharmaceutics	Anticonvulsant	Parent	1
Galaxolide	HHCB	C18H26O	258.40	1222-05-5	Personal Care Product	Polycyclic musks	Parent	41
Gemfibrozil		C15H22O3	250.33	25812-30-0	Pharmaceutics	Lipid-lowering drugs	Parent	306
Glibenclamide		C23H28ClN3O5S	494.00	10238-21-8	Pharmaceutics	Anti-diabetic medications	Parent	37
Haloperidol		C21H23ClFNO2	375.86	52-86-8	Pharmaceutics	Psychiatric medication	Parent	9
Hepta-bromodiphenylether	Hepta-BDE				Industrial Agents	Flame Retardant	Parent	2
Hexabromobiphenyl		C12H4Br6	627.58	59261-08-4	Industrial Agents	Flame retardant	Parent	11
Hexachlorobenzene		C6Cl6	284.78	118-74-1	Pesticide	Fungicide	Parent	6
Hexachlorobutadiene		C4Cl6	260.76	87-68-3	Industrial Agents	Solving Agent	Parent	16
Hexachlorocyclohexane		C6H6Cl6	290.83	119911-70-5	Pesticide	Insecticide	Parent	6
Hexazinone		C12H20N4O2	252.31	51235-04-2	Pesticide	Herbicide	Parent	13
Hydrochlorothiazide		C7H8ClN3O4S2	297.74	58-93-5	Pharmaceutics	Diuretics	Parent	123
Hydrocinnamic acid		C9H10O2	150.18	501-52-0	Personal Care Product	Food Additive, Cosmetics	Parent	4
Hydroxyatrazine		C8H15N5O	197.24	2163-68-0	Pesticide	Pesticide	Parent	1
Hydroxydeethylatrazine				19988-24-0	Pesticide	Pesticide	Transformation Product	1
Hydroxydeisopropylatrazine					Pesticide	Pesticide	Transformation Product	1
Hydroxy-metronidazole		C6H9N3O4	187.15	4812-40-2	Pharmaceutics	Antibiotics	Transformation Product	2
Hydroxyzine		C21H27ClN2O2	374.90	68-88-2	Pharmaceutics	Antihistamine	Parent	8
Ibuprofen		C13H18O2	206.28	15687-27-1	Pharmaceutics	Analgesics	Parent	406
Ifosfamide		C7H15Cl2N2O2P	261.09	3778-73-2	Pharmaceutics	Chemotherapeutic agents	Parent	11
Imipramine		C19H24N2	280.41	50-49-7	Pharmaceutics	Antidepressant	Parent	5
Indenopyrene		C23H14	290.36	193-39-5	Industrial Agents	By-Product of burning Fossils	Transformation Product	2
Indometacine		C19H16ClNO4	357.79	53-86-1	Pharmaceutics	Analgesics	Parent	89
Iodipamide		C20H14I6N2O6	1139.76	606-17-7	Pharmaceutics	Radiocontrast agents	Parent	12
Iohexol		C19H26I3N3O9	821.14	66108-95-0	Pharmaceutics	Radiocontrast agents	Parent	23
Iomeprol		C17H22I3N3O8	777.09	78649-41-9	Pharmaceutics	Radiocontrast agents	Parent	18
Iopamidol		C17H22I3N3O8	777.09	60166-93-0	Pharmaceutics	Radiocontrast agents	Parent	27
Iopromide		C18H24I3N3O8	791.11	73334-07-3	Pharmaceutics	Radiocontrast agents	Parent	53



Substance					Application			Statistics
Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Iothalamic acid		C11H9I3N2O4	613.91	2276-90-6	Pharmaceutics	Radiocontrast agents	Parent	12
Ioxaglic acid		C24H21I6N5O8	1268.88	59017-64-0	Pharmaceutics	Radiocontrast agents	Parent	16
Ioxithalamic acid		C12H11I3N2O5	643.94	96-83-3	Pharmaceutics	Radiocontrast agents	Parent	16
Irbesartan		C25H28N6O	428.53	138402-11-6	Pharmaceutics	Antihypertensives	Parent	39
Isoproturon		C12H18N2O	206.28	34123-59-6	Pesticide	Herbicide	Parent	46
Josamycin		C42H69NO15	827.99	16846-24-5	Pharmaceutics	Antibiotics	Parent	18
Ketoprofen		C16H14O3	254.28	22071-15-4	Pharmaceutics	Analgesics	Parent	224
Ketorolac		C15H13NO3	255.27	74103-06-3	Pharmaceutics	Anti-inflammatory drug	Parent	8
Labetalol		C19H24N2O3	328.41	36894-69-6	Pharmaceutics	Antihypertensives	Parent	5
Lamotrigine		C9H7Cl2N5	256.09	84057-84-1	Pharmaceutics	Anticonvulsant	Parent	4
Lansoprazole		C16H14F3N3O2S	369.36	103577-45-3	Pharmaceutics	Antacids	Parent	14
Levamisole		C11H12N2S	204.29	14769-73-4	Pharmaceutics	Anthelmintics	Parent	14
Levonorgestrel		C21H28O2	312.45	797-63-7	Pharmaceutics	Gestagen	Parent	3
Lincomycin		C18H34N2O6S	406.54	154-21-2	Pharmaceutics	Antibiotics	Parent	30
Linuron		C9H10Cl2N2O2	249.09	330-55-2	Pesticide	Herbicide	Parent	13
Lisinopril		C21H31N3O5	405.49	83915-83-7	Pharmaceutics	Antihypertensives	Parent	10
Lomefloxacin		C17H19F2N3O3	351.35	98079-51-7	Pharmaceutics	Antibiotics	Parent	2
Loratadine		C22H23ClN2O2	382.88	79794-75-5	Pharmaceutics	Antihistamine	Parent	46
Lorazepam		C15H10Cl2N2O2	321.16	846-49-1	Pharmaceutics	Anxiolytics	Parent	89
Losartan		C22H23ClN6O	422.91	114798-26-4	Pharmaceutics	Antihypertensives	Parent	16
Marbofloxacin		C17H19FN4O4	362.36	115550-35-1	Pharmaceutics	Antibiotics	Parent	3
Mecoprop	MCPP	C10H11ClO3	214.65	7085-19-0	Pesticide	Herbicide	Parent	34
Mefenamic acid		C15H15NO2	241.29	61-68-7	Pharmaceutics	Nonsteroidal Anti-inflammatory drug	Parent	80
Meloxicam		C14H13N3O4S2	351.40	71125-39-8	Pharmaceutics	Analgesics	Parent	3
Memantine		C12H21N	179.30	19982-08-2	Pharmaceutics	Anti-dementia agents	Parent	14
Mepivacaine		C15H22N2O	246.35	96-88-8	Pharmaceutics	Anaesthetics	Parent	42
Mestranol		C21H26O2	310.43	72-33-3	Pharmaceutics	Estrogen	Parent	11
Metamizole		C13H17N3O4S	311.36	68-89-3	Pharmaceutics	Analgesics	Parent	1
Metformin		C4H11N5	129.16	657-24-9	Pharmaceutics	Anti-diabetic medications	Parent	6
Methabenzthiazuron		C10H11N3OS	221.28	18691-97-9	Pesticide	Herbicide, Algicide	Parent	13
Methadone		C21H27NO	309.45	76-99-33	Pharmaceutics	Morphine derivates	Parent	4

Substance					Application			Statistics
Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Methyl dihydrojasmonate		C13H22O3	226.31	24851-98-7	Personal Care Product	Fragrance	Parent	8
Methylparaben		C8H8O3	152.15	99-76-3	Personal Care Product	Cosmetics, Washing Agent	Parent	6
Methyltriclosan		C13H9Cl3O2	303.57	4640-01-1	Pharmaceutics	Disinfectants	Transformation Product	1
Metolachlor		C15H22ClNO2	283.79	51218-45-2	Pesticide	Herbicide	Parent	16
Metoprolol		C15H25NO3	267.36	37350-58-6	Pharmaceutics	Beta blockers	Parent	145
Metronidazole		C6H9N3O3	171.15	443-48-1	Pharmaceutics	Antibiotics	Parent	63
Metronidazole-OH		C6H9N3O4	187.15	4812-40-2	Pharmaceutics	Antibiotics	Transformation Product	3
Mevastatin		C23H34O5	390.51	73573-88-3	Pharmaceutics	Lipid-lowering drugs	Parent	15
Mianserin		C18H20N2	264.37	24219-97-4	Pharmaceutics	Antidepressant	Parent	6
Minocycline		C23H27N3O7	457.48	10118-90-8	Pharmaceutics	Antibiotics	Parent	4
Morphine		C17H19NO3	285.34	57-27-2	Pharmaceutics	Morphine derivatives	Parent	4
Moxifloxacin		C21H24FN3O4	401.43	354812-41-2	Pharmaceutics	Antibiotics	Parent	2
Musk ketone		C14H18N2O5	294.30	81-14-1	Personal Care Product	Cosmetics, Fragrance	Parent	6
Musk xylene		C12H15N3O6	297.26	81-15-2	Personal Care Product	Cosmetics, Fragrance	Parent	8
N-(phenylsulfonyl)-sarcosine		C9H11NO4S	229.25	46376-16-3	Industrial Agents	Byproduct	Parent	1
N4-Acetyl sulfamethazine		C14H16N4O3S	320.37	100-90-3	Pharmaceutics	Antibiotics	Transformation Product	20
N4-Acetylsulfamethoxazole		C12H13N3O4S	295.31	21312-10-7	Pharmaceutics	Antibiotics	Transformation Product	4
N-Acetyl sulfadiazine		C12H12N4O3S	292.31	127-74-2	Pharmaceutics	Antibiotics	Transformation Product	5
N-acetyl-4-aminoantipyrine	Ampirone	C13H15N3O2	245.28	83-07-8	Pharmaceutics	Analgesics	Transformation Product	9
N-Acetylsulfamerazine		C13H14N4O3S	306.34	127-73-1	Pharmaceutics	Antibiotics	Product	3
Nadolol		C17H27NO4	309.40	42200-33-9	Pharmaceutics	Beta blockers	Parent	35
Nalidixic acid		C12H12N2O3	232.24	389-08-2	Pharmaceutics	Antibiotics	Parent	6
Naproxen		C14H14O3	230.26	22204-53-1	Pharmaceutics	Analgesics	Parent	406
Napthalene		C10H8	128.16	91-20-3	Personal Care Product	Insecticide	Parent	11
Nefazodone		C25H32ClN5O2	470.01	83366-66-9	Pharmaceutics	Antidepressant	Parent	1
N-formyl-4-aminoantipyrine		C12H13N3O2	231.25	1672-58-8	Pharmaceutics	Analgesics	Transformation Product	32
Nicotine		C10H14N2	162.23	54-11-5	Personal Care Product	Psychoactive Substance	Parent	10
Nifuroxazide		C12H9N3O5	275.22	965-52-6	Pharmaceutics	Antibiotics	Parent	15

Substance					Application			Statistics
Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Nimesulide		C13H12N2O5S	308.31	51803-78-2	Pharmaceutics	Analgesics	Parent	2
Nitrophenol		C6H5NO3	139.11	88-75-5	Industrial Agents	Intermediate in Paint Production, Arms Industry and Pharma Industry	Intermediate	33
N'N'-Diethyltoluamide	DEET	C12H17NO	191.27	134-62-3	Personal Care Product	Insect Repellent	Parent	27
Nonylphenol		C15H24O	220.35	108-95-2	Industrial Agents	Tenside, Plasticizer, Fungicide	Intermediate	46
Nonylphenol diethoxycarboxylate	NP2EC				Industrial Agents	Tenside, Plasticizer, Fungicide	Transformation Product	11
Nonylphenol diethoxylate	NP2EO			26027-38-2	Industrial Agents	Tenside, Plasticizer, Fungicide	Transformation Product	37
Nonylphenol menothoxylate	NP1EO			26027-38-3	Industrial Agents	Tenside, Plasticizer, Fungicide	Transformation Product	15
Nonylphenol monocarboxylate	NP1EC			3115-49-9	Industrial Agents	Tenside, Plasticizer, Fungicide	Transformation Product	35
Nonylphenol-triethoxy-carboxylate	NP3EC				Industrial Agents	Tenside, Plasticizer, Fungicide	Transformation Product	11
norBenzoyllecgonine		C15H17NO4	275.30	60426-41-7	Pharmaceutics	Psychoactive Substance (Drug Abuse)	Transformation Product	3
Nordiazepam		C15H11ClN2O	270.71	1088-11-5	Pharmaceutics	Psychiatric medication	Transformation Product	21
Norethisterone		C20H26O2	298.42	68-22-4	Pharmaceutics	Estrogen	Parent	6
Norfloxacin		C16H18FN3O3	319.33	70458-96-7	Pharmaceutics	Antibiotics	Parent	82
Norfluoxetine		C16H16F3NO	295.30	83891-03-6	Pharmaceutics	Antidepressant	Transformation Product	2
Octamethylcyclotetrasiloxane	D4	C8H24O4Si4	296.62	556-67-2	Personal Care Product	Cosmetics, Washing Agent	Parent	12
Octamethylpentasiloxane	MD3M			144739-99-1	Personal Care Product	Cosmetics	Parent	12
Octamethyltrisiloxane	MDM	C8H24O2Si3	236.53	107-51-7	Personal Care Product	Cosmetics	Parent	12
Octylcrylene		C24H27NO2	361.48	6197-30-4	Personal Care Product	Cosmetics	Parent	2
Octylphenol		C14H22O	206.32	27193-28-8	Industrial Agents	Production of Paint, resign, tire	Intermediate	8
Octylphenol diethoxylate	OP2EO				Industrial Agents	Production of Paint, resign, tire	Transformation Product	7
Octylphenol monocarboxylate	OP1EC				Industrial Agents	Production of Paint, resign, tire	Transformation Product	2
Octylphenol monoethoxylate	OP1EO				Industrial Agents	Production of Paint, resign, tire	Transformation Product	3
Ofloxacin		C18H20FN3O4	361.37	82419-36-1	Pharmaceutics	Antibiotics	Parent	152
Olanzapine		C17H20N4S	312.43	132539-06-1	Pharmaceutics	Neuroleptics	Parent	3
Olaquinox		C12H17N3O4	267.28	23696-28-8	Pharmaceutics	Antibiotics	Parent	3
Oleandomycin		C35H61NO12	687.86	3922-90-5	Pharmaceutics	Antibiotics	Parent	4

Substance					Application			Statistics
Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Omeprazole		C17H19N3O3S	345.42	73590-58-6	Pharmaceutics	Antiulcerants	Parent	21
Orbifloxacin		C19H20F3N3O3	395.38	113617-63-3	Pharmaceutics	Antibiotics	Parent	3
Ornidazole		C7H10ClN3O3	219.63	16773-42-5	Pharmaceutics	Antibiotics	Parent	6
Orphenadrine		C18H23NO	269.38	83-98-7	Pharmaceutics	Antihistamine	Parent	11
Oxacillin		C19H18ClN3O5S	435.88	66-79-5	Pharmaceutics	Antibiotics	Parent	2
Oxazepam		C15H11ClN2O2	286.71	604-75-1	Pharmaceutics	Anxiolytics	Parent	63
Oxolinic acid		C13H11NO5	261.23	14698-29-4	Pharmaceutics	Antibiotics	Parent	8
Oxybenzone		C14H12O3	228.24	131-57-7	Personal Care Product	Cosmetics	Parent	14
Oxytetracycline		C22H24N2O9	460.43	79-57-2	Pharmaceutics	Antibiotics	Parent	28
Pantoprazole		C16H15F2N3O4S	383.37	102625-70-7	Pharmaceutics	Anticulerants	Parent	6
Paracetamol		C8H9NO2	151.16	103-90-2	Pharmaceutics	Analgesics	Parent	185
Parathion-methyl		C8H10NO5PS	263.21	298-00-0	Pesticide	Insectizide, Akarizide	Parent	12
Paraxanthine		C7H8N4O2	180.16	611-59-6	Personal Care Product	Metabolite of Caffeine	Transformation Product	8
Paroxetine		C19H20FNO3	329.37	61869-08-7	Pharmaceutics	Antidepressant	Parent	31
Pefloxacin		C17H20FN3O3	333.36	70458-92-3	Pharmaceutics	Antibiotics	Parent	2
Penta-bromdiphenylether	BDE-47	C12H5Br5O	564.69	32534-81-9	Industrial Agents	Production of Polyethan-Foam	Parent	13
Pentabromobiphenyl		C12H5Br5	548.69	67888-96-4	Industrial Agents	Flame retardant	Parent	11
Pentaclorobenzene		C6HCl5	250.34	608-93-5	Industrial Agents	Production of Benzene, Pesticides,	Intermediate	4
Pentobarbital		C11H18N2O3	226.27	76-74-4	Pharmaceutics	Barbiturates	Parent	4
Pentoxifylline		C13H18N4O3	278.31	6493-05-6	Pharmaceutics	Anti-inflammatory drug	Parent	12
Perflourooctanoate	PFOA	C8F15O2	413.06	355-67-1	Industrial Agents	Emulsifier, Foam Agent, Plasticizer	Parent	46
Perfluorobutansulfonate	PFBS	C4HF9O3S	300.10	375-73-5	Industrial Agents	Emulsifier, Foam Agent, Plasticizer	Parent	14
Perfluorodecanoate	PFDA	C10F19O2	513.08	307-79-9	Industrial Agents	Emulsifier, Foam Agent, Plasticizer	Parent	50
Perfluorododecanoic acid	PFDoA	C12HF23O2	614.10	307-55-1	Industrial Agents	Emulsifier, Foam Agent, Plasticizer	Parent	11
Perfluoroheptanoate	PFHpA	C7F13O2	363.05	375-85-9	Industrial Agents	Emulsifier, Foam Agent, Plasticizer	Parent	48
Perfluorohexanoate	PFHxA	C6F11O2	313.05	307-24-4	Industrial Agents	Emulsifier, Foam Agent, Plasticizer	Parent	36
Perfluorohexane sulfonate	PFHxS	C6HF13O3S	399.11	432-50-7	Industrial Agents	Emulsifier, Foam Agent, Plasticizer	Parent	14
Perfluorononanoate	PFNA	C9F17O2	463.07	375-95-1	Industrial Agents	Emulsifier, Foam Agent, Plasticizer	Parent	47
Perfluorooctane sulfonate	PFOS	C8HF17O3S	500.13	45298-90-6	Industrial Agents	Emulsifier, Foam Agent, Plasticizer	Parent	47
Perfluoropentanoic acid	PFPeA	C5HF9O2	264.05	2706-90-3	Industrial Agents	Production of Pesticides	Intermediate	3
Perfluoroundecanoic acid	PFUnA	C11HF21O2	564.09	2058-94-8	Industrial Agents	Emulsifier, Foam Agent, Plasticizer	Parent	31

Substance					Application			Statistics
Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Phantolid	AHMI	C17H24O	244.37	15323-35-0	Personal Care Product	Cosmetics, Musk Fragrances	Parent	12
Phenacetin		C10H13NO2	179.22	62-44-2	Pharmaceutics	Anti-inflammatory drug	Parent	12
Phenanthrene		C14H10	178.23	85-01-8	Industrial Agents	Paint Production	Intermediate	9
Phenazone		C11H12N2O	188.23	60-80-0	Pharmaceutics	Analgesics	Parent	83
Phenobarbital		C12H12N2O3	232.23	50-06-6	Pharmaceutics	Anticonvulsant	Parent	8
Phenoxyethylpenicillin		C16H18N2O5S	350.39	87-08-1	Pharmaceutics	Antibiotics	Parent	4
Phenylbutazone		C19H20N2O2	308.37	50-33-9	Pharmaceutics	Nonsteroidal Anti-inflammatory drug	Parent	8
Phenytoin		C15H12N2O2	252.27	57-41-0	Pharmaceutics	Antiepileptic drugs	Parent	6
Pindolol		C14H20N2O2	248.32	13523-86-9	Pharmaceutics	Beta blockers	Parent	18
Pipemidic acid		C14H17N5O3	303.32	51940-44-4	Pharmaceutics	Antibiotics	Parent	5
Piroxicam		C15H13N3O4S	331.35	36322-90-4	Pharmaceutics	Analgesics	Parent	4
Pizotifen		C19H21NS	295.44	15574-96-6	Pharmaceutics	Anti-migraine agents	Parent	2
Pravastatin		C23H36O7	424.53	81093-37-0	Pharmaceutics	Lipid-lowering drugs	Parent	60
Primidone		C12H14N2O2	218.25	125-33-7	Pharmaceutics	Anticonvulsant	Parent	28
Procymidone		C13H11Cl2NO2	284.14	32809-16-8	Pesticide	Fungicide	Parent	6
Progesterone		C21H30O2	314.46	57-83-0	Pharmaceutics	Progestogen	Parent	4
Propazine		C9H16ClN5	229.71	139-40-2	Pesticide	Pesticide	Parent	3
Propranolol		C16H21NO2	259.34	525-66-6	Pharmaceutics	Beta blockers	Parent	191
Propylparaben		C10H12O3	180.20	94-13-3	Pharmaceutics	Preservative	Parent	8
Propyphenazone		C14H18N2O	230.31	479-92-5	Pharmaceutics	Analgesics	Parent	104
Pyrene		C16H10	202.25	129-00-0	Industrial Agents	Production of dyes and dyes precursors	Intermediate	3
Ranitidine		C13H22N4O3S	314.40	66357-35-5	Pharmaceutics	Antihistamine	Parent	133
Ranitidine-N-Oxide		C13H22N4O4S	330.40	73857-20-2	Pharmaceutics	Antihistamine	Transformation Product	4
Repaglinide		C27H36N2O4	452.59	135062-02-1	Pharmaceutics	Anti-diabetic medications	Parent	14
Rifampicin		C43H58N4O12	822.94	13292-46-1	Pharmaceutics	Antibiotics	Parent	1
Risperidone		C23H27FN4O2	410.48	106266-06-2	Pharmaceutics	Neuroleptics	Parent	14
Rosuvastatin		C22H28FN3O6S	481.54	287714-41-4	Pharmaceutics	Statins	Parent	4
Roxithromycin		C41H76N2O15	837.05	80214-83-1	Pharmaceutics	Antibiotics	Parent	55
Saccharine		C7H5NO3S	183.19	81-07-2	Food Additives	Sweetener	Parent	11
Salbutamol		C13H21NO3	239.31	18559-94-9	Pharmaceutics	Anti-asthmatics	Parent	63
Salicylic acid		C7H6O3	138.12	69-72-7	Pharmaceutics	Natural product	Parent	136

Substance					Application			Statistics
Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Sarafloxacin		C20H17F2N3O3	385.36	98105-99-8	Pharmaceutics	Antibiotics	Parent	3
Sertraline		C17H17Cl2N	306.23	79617-96-2	Pharmaceutics	Antidepressant	Parent	1
Sildenafil		C22H30N6O4S	474.58	139755-83-2	Pharmaceutics	PDE-5-Blocker	Parent	4
Simazine		C7H12ClN5	201.66	122-34-9	Pesticide	Herbicide	Parent	48
Simvastatin		C25H38O5	418.57	79902-63-9	Pharmaceutics	Lipid-lowering drugs	Parent	8
Sotalol		C12H20N2O3S	272.36	3930-20-9	Pharmaceutics	Beta blockers	Parent	112
Spiramycin		C43H74N2O14	8043.05	8025-81-8	Pharmaceutics	Antibiotics	Parent	44
Succinylsulfathiazole		C13H13N3O5S2	355.39	116-43-8	Pharmaceutics	Antibiotics	Parent	6
Sucralose		C12H19Cl3O8	397.63	56038-13-2	Food Additives	Sweetener	Parent	14
Sulfabenzamide		C13H12N2O3S	276.31	127-71-9	Pharmaceutics	Antibiotics	Parent	13
Sulfadiazine		C10H10N4O2S	250.28	68-35-9	Pharmaceutics	Antibiotics	Parent	71
Sulfadimethoxine		C12H14N4O4S	310.33	122-11-2	Pharmaceutics	Antibiotics	Parent	28
Sulfadimidine		C12H14N4O2S	278.33	57-68-1	Pharmaceutics	Antibiotics	Parent	14
Sulfadoxine		C12H14N4O4S	310.33	2447-57-6	Pharmaceutics	Antibiotics	Parent	10
Sulfamerazine		C11H12N4O2S	264.30	127-79-7	Pharmaceutics	Antibiotics	Parent	13
Sulfamethazine		C12H14N4O2S	278.33	57-68-1	Pharmaceutics	Antibiotics	Parent	91
Sulfamethizole		C9H10N4O2S2	270.33	144-82-1	Pharmaceutics	Antibiotics	Parent	16
Sulfamethoxazole		C10H11N3O3S	25.28	723-46-6	Pharmaceutics	Antibiotics	Parent	392
Sulfamethoxazolepyridazine		C11H12N4O3S	280.30	80-35-3	Pharmaceutics	Antibiotics	Parent	16
Sulfanitran		C14H13N3O5S	335.34	122-16-7	Pharmaceutics	Antibiotics	Parent	8
Sulfapyridine		C11H11N3O2S	249.29	144-83-2	Pharmaceutics	Antibiotics	Parent	59
Sulfaquinoxaline		C14H12N4O2S	300.34	59-40-5	Pharmaceutics	Antibiotics	Parent	10
Sulfathiazole		C9H9N3O2S2	255.32	72-14-0	Pharmaceutics	Antibiotics	Parent	22
Sulfisomidine		C12H14N4O2S	278.33	515-65-0	Pharmaceutics	Antibiotics	Parent	10
Sulfisoxazole		C11H13N3O3S	267.30	127-69-5	Pharmaceutics	Antibiotics	Parent	17
Tamoxifen		C26H29NO	371.52	10540-29-1	Pharmaceutics	Selective estrogen receptor modulators	Parent	14
Tamsulosin		C20H28N2O5S	408.51	106133-20-4	Pharmaceutics	Alpha blockers	Parent	2
Telmisartan		C33H30N4O2	514.62	144701-48-4	Pharmaceutics	Antihypertensives	Parent	14
Tenoxicam		C13H11N3O4S2	337.37	59804-37-4	Pharmaceutics	Analgesics	Parent	1
Terbinafine		C21H25N	291.43	91161-71-6	Pharmaceutics	Antifungal medication	Parent	1
Terbutaline		C12H19NO3	225.28	23031-25-6	Pharmaceutics	Anti-asthmatics	Parent	13

Substance					Application			Statistics
Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Terbutylazine		C9H16CIN5	229.71	5915-41-3	Pesticide	Herbicide	Parent	12
Terbutryn		C10H19N5S	241.36	886-50-0	Industrial Agents	Algicide	Parent	14
Terbutyl phosphate		C12H27O4P	266.31	126-73-8	Industrial Agents	Solvent, Plasticizer	Parent	4
Terbutylazine		C9H16CIN5	229.70	5915-41-3	Pesticide	Herbicide	Parent Transformation	30
Tert-Nonylphenol		C15H24O	220.35	84852-15-3	Industrial Agents	Washing Agent	Product	8
Tert-Octylphenol		C14H22O	206.33	140-66-9	Industrial Agents	Production of resin and tyre	Intermediate	34
Testosterone		C19H28O2	288.43	58-22-0	Pharmaceutics	Androgen	Parent	9
Tetrabromobiphenyl	Tetra-BDE	C12H6Br4	469.79	60044-24-8	Industrial Agents	Flame retardant	Parent	15
Tetra-bromodiphenyl ether	BDE-77			5436-43-1	Industrial Agents	Flame retardant	Parent	6
Tetracycline		C22H24N2O8	444.44	60-54-8	Pharmaceutics	Antibiotics	Parent	44
Thiabendazole		C10H7N3S	201.25	148-79-8	Pharmaceutics	Anthelmintics	Parent	7
Tiamulin		C28H47NO4S	493.74	55297-95-5	Pharmaceutics	Antibiotics	Parent	3
Tilmicosin		C46H80N2O13	869.13	108050-54-0	Pharmaceutics	Antibiotics	Parent	7
Timolol		C13H24N4O3S	316.42	26839-75-8	Pharmaceutics	Beta blockers	Parent	33
Tolytriazole		C7H7N3	133.15	29385-43-1	Industrial Agents	Anticorrosive	Parent	7
Tonalid	AHTN	C18H26O3	258.40	21145-77-7	Personal Care Product	Cosmetics, Musk Fragrances	Parent	33
Torasemide		C16H20N4O3S	348.42	56211-40-6	Pharmaceutics	Diuretics	Parent	5
Total Bromodiphenyl	BDE-SUM				Industrial Agents	Flame retardant	Parent	11
Traesolid	ATII	C18H26O	258.40	68140-48-7	Personal Care Product	Cosmetics, Musk Fragrances	Parent	12
Tramadol		C16H25NO2	263.38	27203-92-5	Pharmaceutics	Analgesics	Parent	14
Trans-Chlorfenvinphos		C12H14Cl3O4P	359.57	470-90-6	Pesticide	Insecticide	Parent	3
Trazodone		C19H22CIN5O	371.86	19794-93-5	Pharmaceutics	Antidepressant	Parent	5
Tri(2-chloroethyl)phosphate		C6H12Cl3O4P	285.49	115-96-8	Industrial Agents	Plasticizer, Flame retardant	Parent	8
Triamcinolone		C21H27FO6	394.43	124-94-7	Pharmaceutics	Glucocorticoids	Parent	1
Triamcinolone acetoneide		C24H31FO6	434.50	76-25-5	Pharmaceutics	Glucocorticoids	Parent	1
Tribromobiphenyl		C12H7Br3	390.90	59080-35-2	Industrial Agents	Flame retardant	Parent	11
Tributyl phosphate		C12H27O4P	266.31	126-73-8	Industrial Agents	Solvent, Plasticizer	Parent	4
Tributylphosphate	TBP	C12H27O4P	266.31	6131-90-4	Industrial Agents	Flame retardant	Parent	14
Triclosan		C12H7Cl3O2	289.54	3380-34-5	Pharmaceutics	Disinfectants	Parent	139
Tricresylphosphate	TCP	C12H7Cl3O2	289.54	1330-78-5	Industrial Agents	Flame retardant	Parent	14
Trifluralin		C13H16F3N3O4	335.28	1582-09-8	Pesticide	Herbicide	Parent	2

Substance					Application			Statistics
Name	Short Name	Formula	Mass [g/mol]	CAS	Sector	Specific Application	Type	Nb of data
Trihexyphenidyl		C20H31NO	301.47	144-11-6	Pharmaceutics	Anti-dementia agents	Parent	9
Tri-iso-butylphosphate	TIBP	C12H27O4P	266.31	126-71-6	Industrial Agents	Flame Retardant, Solvent, Antifoam	Parent	14
Trimethoprim		C14H18N4O3	290.32	738-70-5	Pharmaceutics	Antibiotics	Parent	213
Triphenylphosphate	TPP	C18H15O4P	326.28	115-86-6	Industrial Agents	Flame retardant	Parent	14
Tris(1,3-dichloro-2-propyl)phosphate	TDCP	C9H15Cl6O4P	430.91	13674-87-8	Industrial Agents	Flame retardant	Parent	26
Tris(2-butoxyethyl)phosphate	TBEP	C18H39O7P	398.47	126-73-8	Industrial Agents	Flame retardant	Parent	18
Tris(2-chlorethyl)phosphate	TCEP	C6H12Cl3O4P	285.49	115-96-8	Industrial Agents	Flame retardant, Plasticizer	Parent	27
Tris(2-chloroisopropyl)phosphate	TCPP	C9H18Cl3O4P	327.57	115-96-8	Industrial Agents	Flame retardant, Plasticizer	Parent	39
Tris(2-ethylhexyl)phosphate	TEHP	C24H51O4P	434.63	78-42-2	Industrial Agents	Flame retardant	Parent	14
Tylosin		C46H77NO17	916.10	1401-69-0	Pharmaceutics	Antibiotics	Parent	31
Valsartan		C24H29N5O3	435.52	137862-53-4	Pharmaceutics	Antihypertensives	Parent	25
Vancomycin		C66H75Cl2N9O24	1449.25	1404-90-6	Pharmaceutics	Antibiotics	Parent	2
Venlafaxine		C17H27NO2	277.40	93413-69-5	Pharmaceutics	Antidepressant	Parent	82
Verapamil		C27H38N2O4	454.60	52-53-9	Pharmaceutics	Antihypertensives	Parent	3
Warfarin		C19H16O4	308.33	81-81-2	Pharmaceutics	Anticoagulant	Parent	3
Xylazine		C12H16N2S	220.33	7361-61-7	Pharmaceutics	Sedatives	Parent	4
Zolpidem		C19H21N3O	307.39	82626-48-0	Pharmaceutics	Hypnotics	Parent	10
Beta-Sitosterol		C29H50O	414.69	83-46-5	Pharmaceutics (Food additives)	Lipid-lowering drugs	Parent	11