

Known contact allergens.

For toxicity and effect values, consult TerraTox™ databases, or TerraBase Inc.

CAS	EINECS	RTECS	Name	SMILES	Formula	MW
50-00-0	200-001-8	LP 8925000	formaldehyde; methanal	O=C	CH2O	30.03
107-22-2	203-474-9	MD 2700000	glyoxal	O=CC=O	C2H2O2	58.04
68-11-1	200-677-4	AI 5950000	mercaptoacetic acid; thioglycolic acid	O=C(O)CS	C2H4O2S	92.11
70-25-7	200-730-1	MF 4200000	N-methyl-N'-nitro-N-nitrosoguanidine	O=N(=O)NC(=N)N(N=O)C	C2H5N5O3	147.09
96-50-4	202-511-6	XJ 2100000	2-aminothiazole	s1c(N)ncc1	C3H4N2S	100.14
106-89-8	203-439-8	TX 4900000	epichlorohydrin	O(C1CC)C1	C3H5ClO	92.52
2832-19-1	220-598-9	AB 5733000	acetamide, 2-chloro-N-(hydroxymethyl)-; N-methylol chloroacetamide	ClCC(=O)NCO	C3H6ClNO2	123.54
96-45-7	202-506-9	NI 9265000	ethylenethiourea; ETU	N(C(=S)NC1)C1	C3H6N2S	102.15
57-06-7	200-309-2	NX 8225000	allyl isothiocyanate	N(=C=S)CC=C	C4H5NS	99.15
111-42-2	203-868-0	KL 2975000	diethanolamine	OCCNCCO	C4H11NO2	105.14
111-40-0	203-865-4	IE 1225000	diethylenetriamine	N(CCN)CCN	C4H13N3	103.17
5451-40-1	226-681-6		2,6-dichloropurine	Clc1nc(Cl)nc2ncnc12	C5H2Cl2N4	189.00
98-01-1	202-627-7	LT 7000000	2-furaldehyde; furfural	O=Cc(Occ1)c1	C5H4O2	96.09
547-65-9			2-methylene-4-butyrolactone	C=C1C(=O)OCC1	C5H6O2	98.10
T-4735-003			2-chloro-4-nitro-6-cyanopyridine	n1c(Cl)cc(N(=O)=O)cc1C#N	C6H2ClN3O2	183.55
88-88-0	201-864-3	CZ 1225900	picryl chloride	Clc1c(N(=O)=O)cc(N(=O)=O)cc1N(=O)=O	C6H2ClN3O6	247.55
97-00-7	202-551-4	CZ 0525000	1-chloro-2,4-dinitrobenzene	O=N(=O)c(ccc(c1N(=O)=O)Cl)c1	C6H3ClN2O4	202.55
106-51-4	203-405-2	DK 2625000	1,4-benzoquinone	C1(=O)C=CC(=O)C=C1	C6H4O2	108.10
59-87-0	200-443-1	LT 7700000	nitrofurazone; 5-nitro-2-furaldehyde semicarbazone	o1c(N(=O)=O)ccc1/C=N/NC(=O)N	C6H6N4O4	198.14
123-31-9	204-617-8	MX 3500000	hydroquinone	Oc(ccc(O)c1)c1	C6H6O2	110.11
501-30-4	207-922-4	UQ 0875000	kojic acid	O1C=C(O)C(=O)C=C1CO	C6H6O4	142.11
62-53-3	200-539-3	BW 6650000	aniline	Nc(cccc1)c1	C6H7N	93.13
591-27-5	209-711-2	SJ 4900000	3-aminophenol	Oc(cccc1N)c1	C6H7NO	109.13
106-50-3	203-404-7	SS 8050000	1,4-phenylenediamine	Nc(ccc(N)c1)c1	C6H8N2	108.14
95-86-3		SK 7530000	2,4-diaminophenol	c1cc(N)cc(N)c1O	C6H8N2O	124.14
868-77-9	212-782-2	OZ 4725000	2-hydroxyethyl methacrylate	O=C(OCCO)C(=C)C	C6H10O3	130.14
137-26-8	205-286-2	JD 1400000	Thiram; tetramethylthiuram disulfide	N(C(=S)SSC(N(C)C)=S)(C)C	C6H12N2S4	240.43
6064-63-7			2-hydroxy-n-hexanoic acid; alpha-hydroxycaproic acid	CCCCC(O)C(=O)O	C6H12O3	132.16
106-69-4	203-424-6	MO 4650000	1,2,6-hexanetriol	OCC(O)CCCCO	C6H14O3	134.18
103-71-9	203-137-6	DA 3675000	phenyl isocyanate	O=C=Nc(cccc1)c1	C7H5NO	119.12
103-72-0	203-138-1	NX 9275000	phenyl isothiocyanate	N(c(cccc1)c1)=C=S	C7H5NS	135.18
149-30-4	205-736-8	DL 6475000	2-mercaptobenzothiazole	N(c(c(S1)ccc2)c2)=C1S	C7H5NS2	167.24
123-08-0	204-599-1	CU 6475000	4-hydroxybenzaldehyde	O=Cc(O)ccc1c1	C7H6O2	122.12
99-96-7	202-804-9	DH 1925000	4-hydroxybenzoic acid	O=C(O)c(O)ccc1c1	C7H6O3	138.12
59-50-7	200-431-6	GO 7100000	4-chloro-3-methylphenol	Oc(ccc(c1Cl)c1)c1	C7H7ClO	142.58
100-51-6	202-859-9	DN 3150000	benzyl alcohol	OCC(cccc1)c1	C7H8O	108.14
18829-55-5		MJ 8795000	trans-2-hepten-1-al	O=C/C=C/CCCC	C7H12O	112.17
85-44-9	201-607-5	TI 3150000	phthalic anhydride	O=C(OC(=O)c1ccccc2)c12	C8H4O3	148.12
99-81-0			4-nitrophenacyl bromide	c1cc(N(=O)=O)ccc1C(=O)CBr	C8H6BrNO3	244.05
99-73-0	202-783-6	AM 6950000	4-bromophenacyl bromide	c1cc(Br)ccc1C(=O)CBr	C8H6Br2O	277.95
120-57-0	204-409-7	TO 1575000	heliotropine; piperonal	O=Cc(O)ccc1c(O)ccc12	C8H6O3	150.13
140-29-4	205-410-5	AM 1400000	benzyl cyanide; phenylacetonitrile	N#CCc(cccc1)c1	C8H7N	117.15
86-54-4			hydralazine	c1cccc2c(NN)nncc12	C8H8N4	160.18
122-78-1	204-574-5	CY 1420000	phenylacetaldehyde	O=CCc(cccc1)c1	C8H8O	120.15
6248-20-0	228-369-5		2,4-dihydroxy-3-methylbenzaldehyde	Oc1c(C)c(O)ccc1C=O	C8H8O3	152.15

99-76-3	202-785-7	DH 2450000	methyl 4-hydroxybenzoate; methyl paraben	<chem>O=C(OC)c(O)c1ccccc1</chem>	C8H8O3	152.15
138-89-6	205-343-1	BX 7175000	N,N-dimethyl-4-nitrosoaniline	<chem>O=Nc1ccc(N(C)C)c1</chem>	C8H10N2O	150.18
2937-59-9	220-919-2		2,6-dimethylol-phenol	<chem>Oc1c(CO)cccc1CO</chem>	C8H10O3	154.16
141-05-9	205-451-9	ON 1225000	diethyl maleate	<chem>O=C(OCC)C([H])=C([H])C(=O)OCC</chem>	C8H12O4	172.18
623-91-6	210-819-7	EM 5950000	diethyl 2-butenedioate (E); diethyl fumarate	<chem>O=C(OCC)C=CC(=O)OCC</chem>	C8H12O4	172.18
18318-83-7		MP 6746000	trans-2-hexenal dimethylacetal	<chem>O(C(OC)/C=C/CCC)C</chem>	C8H16O2	144.21
130-26-7		VC 5075000	Vioform	<chem>Oc1c(I)cc(Cl)c2cccnc12</chem>	C9H5ClINO	305.50
56-57-5	200-281-1	VC 2100000	4-nitroquinoline 1-oxide	<chem>O=N(=O)c1cc[n+]{[O-]}c2ccccc12</chem>	C9H6N2O3	190.16
133-06-2	205-087-0	GW 5075000	Captan; 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]-1H-isoindole-1,3(2H)-dione	<chem>O=C(N(SC(Cl)(Cl)Cl)C(=O)C1CC=C(C2)C12</chem>	C9H8Cl3NO2S	300.59
104-55-2	203-213-9	GD 6475000	3-phenylprop-2-enal; cinnamaldehyde	<chem>c1ccccc1/C=C/C=O</chem>	C9H8O	132.16
119-84-6	204-354-9	MW 5775000	dihydrocoumarin	<chem>O=C(Oc(c(O)C)C)C1=CC=CC=C1</chem>	C9H8O2	148.16
104-54-1	203-212-3	GE 2200000	cinnamyl alcohol; 3-phenyl-2-propene-1-ol	<chem>OCC=Cc1ccccc1</chem>	C9H10O	134.18
111-12-6	203-836-6	RI 2735000	methyl 2-octynoate; methyl heptine carbonate	<chem>O=C(OC)C#CCCCC</chem>	C9H14O2	154.21
101-39-3	202-938-8	GD 6600000	alpha-methylcinnamaldehyde	<chem>O=C/C(=C/c1ccccc1)C</chem>	C10H10O	146.19
122-57-6	204-555-1	EN 0330000	methyl styryl ketone; 4-phenyl-but-3-en-2-one; benzylideneacetone	<chem>O=C(/C=C/c1ccccc1)C</chem>	C10H10O	146.19
13443-29-3		DG 9850000	benzoic acid, 2,3-epoxypropyl ester; glycidyl benzoate	<chem>c1ccccc1C(=O)OCC2CO2</chem>	C10H10O3	178.19
97-53-0	202-589-1	SJ 4375000	2-methoxy-4-(2-propenyl)phenol; eugenol; 4-allyl-2-methoxyphenol	<chem>Oc(c(O)ccc1CC=C)c1C</chem>	C10H12O2	164.20
97-54-1	202-590-7	SL 7875000	2-methoxy-4-(1-propenyl)phenol; isoeugenol, cis/trans	<chem>Oc(c(O)ccc1C=CC)c1C</chem>	C10H12O2	164.20
121-79-9	204-498-2	LW 8400000	gallic acid n-propyl ester	<chem>O=C(OCCC)c(O)c(O)c1O)c1</chem>	C10H12O5	212.20
98-54-4	202-679-0	SJ 8925000	4-tert-butylphenol	<chem>Oc(ccc1C)C(C)(C)C1</chem>	C10H14O	150.22
2785-87-7	220-499-0	SL 8050000	dihydroeugenol; 2-methoxy-4-propylphenol; 4-propylguaiaicol	<chem>c1c(CCC)ccc(O)c1OC</chem>	C10H14O2	166.22
1070-70-8	213-979-6	UD 3130000	butane-1,4-diol diacrylate	<chem>C=CC(=O)OCCCCOC(=O)C=C</chem>	C10H14O4	198.22
97-90-5	202-617-2	OZ 4400000	ethyleneglycol dimethacrylate	<chem>O=C(OCCOC(=O)C(=C)C(=C)C</chem>	C10H14O4	198.22
5989-27-5	227-813-5	GW 6360000	D-limonene; (4R)-(+)-limonene	<chem>C(=CC[C@H](C(=C)C)C1)(C1)C</chem>	C10H16	136.24
5392-40-5	226-394-6	RG 5075000	citral [mixture of cis- and trans-3,7-dimethyl-2,6-octadienal]	<chem>O=CC=C(CCC=C(C)C)C</chem>	C10H16O	152.24
106-24-1	203-377-1	RG 5830000	geraniol; 3,7-dimethyl-(E)-2,7-octadien-1-ol; 2-trans-3,7-dimethyl-2,6-octadien-1-ol	<chem>[H]/C(CO)=C(C)\CC/C=C(C)/C</chem>	C10H18O	154.25
121-75-5	204-497-7	WM 8400000	Malathion; Carbofos; dithiophosphoric acid, O,O-dimethyl-S-(1,2-dicarbethoxyethyl) ester	<chem>CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC</chem>	C10H19O6PS2	330.35
106-22-9	203-375-0	RH 3400000	citronellol; 3,7-dimethyl-6-octen-1-ol; 3,7-dimethyloct-6-en-1-ol; CAS also 26489-01-0	<chem>OCC[C@@H](C)CC/C=C(C)/C</chem>	C10H20O	156.27
107-75-5	203-518-7	RG 7850000	3,7-dimethyl-7-hydroxyoctanal; hydroxycitronellal	<chem>CC(O)(C)CCCC(C)CC=O</chem>	C10H20O2	172.27

67746-30-9		MP 6740000	trans-2-hexenal diethyl acetal	<chem>O(C(OCC)/C=C/CCC)CC</chem>	C10H20O2	172.27
93-15-2	202-223-0	CY 2450000	4-allyl-1,2-dimethoxybenzene; methyleugenol	<chem>O(c(c(OC)cc(c1)CC=C)c1)C</chem>	C11H14O2	178.23
T-4735-001			ethylidene heptanoate acetate	<chem>CCCCCCC(=O)OCCOC(=O)C</chem>	C11H20O4	216.28
101-54-2	202-951-9	ST 3150000	4-aminodiphenylamine	<chem>N(c(ccc(N)c1)c1)c(cccc2)c2</chem>	C12H12N2	184.24
534-85-0	208-606-9		2-aminodiphenylamine	<chem>c1ccccc1Nc2ccccc2N</chem>	C12H12N2	184.24
104-27-8		SB 3927000	4-(4-methoxyphenyl)-pent-1-en-3-one	<chem>c1cc(OC)ccc1/C=C/C(=O)CC</chem>	C12H14O2	190.24
2437-25-4	219-440-1	JR 2600000	dodecanonitrile; n-undecyl cyanide	<chem>N#CCCCCCCCCCCC</chem>	C12H23N	181.32
T-4735-009			1,3-dodecanesultone	<chem>O=S(=O)(O1)C(CC1)CCCCCCCCC</chem>	C12H24O3S	248.39
70-30-4	200-733-8	SM 0700000	Hexachlorophene	<chem>Oc(c(c(c(c1)Cl)Cl)Cc(c(c(cc2Cl)Cl)Cl)c2O)c1Cl</chem>	C13H6Cl6O2	406.91
T-4735-008			3,5,3',5'-tetrachlorosalicylanilide	<chem>c1c(Cl)cc(Cl)cc1C(=O)Nc2cc(Cl)cc(Cl)c2</chem>	C13H7Cl4NO	335.02
131-55-5	205-028-9	DJ 1892000	benzophenone, 2,2',4,4'-tetrahydroxy-Monobenzene; 4-	<chem>O=C(c(c(O)cc(O)c1)c1)c(c(O)cc(O)c2)c2</chem>	C13H10O5	246.22
103-16-2	203-083-3	SJ 7700000	(benzyloxy)phenol; hydroquinone O-benzyl ether	<chem>O(c(ccc(O)c1)c1)Cc(cccc2)c2</chem>	C13H12O2	200.24
59-46-1		DG 2100000	procaine	<chem>O=C(OCCN(CC)CC)c(ccc(N)c1)c1</chem>	C13H20N2O2	236.31
141-10-6	205-457-1	YQ 2833700	pseudoionone; 2,6-dimethylundeca-2,6,8-trien-10-one; 6,10-dimethyl-3,5,9-undecatrien-2-one	<chem>O=C(/C=C/C=C(CC/C=C(C)/C)\C)C</chem>	C13H20O	192.30
4756-19-8			cyclamen alcohol; alpha-methyl-p-isopropylhydrocinnamic alcohol	<chem>CC(C)c1cc(ccc1)CC(C)CO</chem>	C13H20O	192.30
26087-47-8	247-449-0	TE 6550000	lprobenfos; kitazin P	<chem>CC(C)OP(=O)(OC(C)C)SCc1ccccc1</chem>	C13H21O3PS	288.34
538-75-0	208-704-1	FF 2160000	1,3-dicyclohexylcarbodiimide	<chem>N(=C=NC(CCCC1)C1)C(CCCC2)C2</chem>	C13H22N2	206.33
31906-04-4	250-863-4	GW 2850000	4-(4-hydroxy-4-methylpentyl)cyclohex-3-enecarboxaldehyde	<chem>O=CC(CCC(=C1)CCCC(O)(C)C)C1</chem>	C13H22O2	210.32
34131-99-2		QK 4240500	6-isopropyl-2-decalol; decahydro-6-(1-methylethyl)-naphthalen-2-ol	<chem>C1CC(C(C)C)CC2CCCC(O)C12</chem>	C13H24O	196.33
31810-89-6		CB 0180000	Disperse Blue 56/2	<chem>O=C1c2c(c(cc(c2C(=O)c3c1c(ccc3N)O)O)Br)N</chem>	C14H9BrN2O4	349.14
T-1573-002			Disperse Blue 56/3	<chem>O=C1c2c(c(cc(c2C(=O)c3c1c(ccc3N)O)O)Cl)N</chem>	C14H9ClN2O4	304.69
115-32-2	204-082-0	DC 8400000	p,p'-Dicofol; Kelthane	<chem>OC(c1ccc(Cl)cc1)(c2ccc(Cl)cc2)C(Cl)(Cl)Cl</chem>	C14H9Cl5O	370.49
116-85-8		CB 5600000	Disperse Red 15; CI 60710; 1-amino-4-hydroxy-9,10-anthraquinone	<chem>O=C(c(c(C(=O)c1c(N)ccc2O)ccc3)c3)c12</chem>	C14H9NO3	239.23
120-51-4	204-402-9	DG 4200000	benzyl benzoate	<chem>O=C(OCc(cccc1)c1)c(cccc2)c2</chem>	C14H12O2	212.25
118-58-1	204-262-9	VO 1750000	benzyl salicylate	<chem>O=C(OCc(cccc1)c1)c(c(O)ccc2)c2</chem>	C14H12O3	228.25
17804-35-2	241-775-7	DD 6475000	Benomyl	<chem>O=C(OC)N=C(N(c(c1ccc2)c2)C(=O)NCCCC)N1</chem>	C14H18N4O3	290.32
122-40-7	204-541-5	GD 6825000	alpha-pentylcinnamaldehyde, cis/trans mixture	<chem>c1ccccc1/C=C(C=O)/CCCC</chem>	C14H18O	202.30
101-85-9	202-982-8	MJ 3280000	1-heptanol, 2-benzylidene-lilial; 2-(4-tert-butylbenzyl)propionaldehyde; lilestralis lilial	<chem>OCC(=Cc(cccc1)c1)CCCC</chem>	C14H20O	204.31
80-54-6	201-289-8	MW 4895000		<chem>O=CC(C)Cc(ccc(c1)C(C)(C)C)c1</chem>	C14H20O	204.31

4493-18-9		XH 8953000	amylpenicillin; penicillin DF	CCCCC(=O)N[C@]1([H])C(=O)N2[C@@]([H])(C(=O)O)C(C)(C)S[C@]12[H]	C14H22N2O4S	314.40
127-51-5	204-846-3		cetone alpha; 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl-3-buten-2-one	O=C(C(=CC(C(=CCC1)C)C1(C)C)C)C	C14H22O	206.33
82-38-2	201-417-2	CB 0536600	Disperse Red 9; CI 60505; 1-methylamino-9,10-anthraquinone	O=C(c(c(c(NC)cc1)C(=O)c2cccc3)c1)c23	C15H11NO2	237.26
2379-90-0	219-170-4	CB 5720000	Disperse Red 4; 9,10-anthraquinone, 1-amino, 2-methoxy, 4-hydroxy	Oc3cc2c(c(c3OC)N)C(=O)c1c(cccc1)C2=O	C15H11NO4	269.26
2872-48-2		CB 6485000	Disperse Red 11; CI 62015	O=C(c(c(C(=O)c1c(N)cc(OC)c2N)cc3)c3)c12	C15H12N2O3	268.27
101-72-4	202-969-7	ST 2650000	N-phenyl-N'-isopropyl-1,4-phenylenediamine	N(c(ccc(Nc(cccc1)c1)c2)c2)C(C)C	C15H18N2	226.32
101-86-0	202-983-3	GD 6560000	alpha-hexyl cinnamaldehyde	O=CC(=Cc(cccc1)c1)CCCCC	C15H20O	216.32
546-43-0			alantolactone	C[C@H]1CCC[C@]2(C)C[C@@]3([H])OC(=O)C(=C)[C@@]3([H])C=C12	C15H20O2	232.32
20554-84-1		LY 4220000	parthenolide	C[C@@]23CC/C=C(/C)CC[C@@]1([H])C(=C)C(=O)O[C@]1([H])[C@@]2([H])O3	C15H20O3	248.32
3600-95-1			perezone; 2,5-cyclohexadiene-1,4-dione, 2-(1,5-dimethyl-4-hexenyl)-3-hydroxy-5-methyl-, (R)-	O=C1C(C)=CC(=O)C([C@H](C)CC/C=C(C)/C)=C1O	C15H20O3	248.32
4602-84-0	225-004-1	JR 4979000	farnesol	OCC=C(CCC=C(CCC=C(C)C)C)C	C15H26O	222.37
90-30-2		QM 4500000	N-phenyl-1-naphthylamine	c1cccc2c1cccc2Nc1cccc1	C16H13N	219.29
2475-44-7	219-602-1	CB 5750000	Disperse Blue 14; CI 61500; 9,10-anthraquinone, 1,4-di(methylamino)	CNc3ccc(c2c3C(=O)c1c(cccc1)C2=O)NC	C16H14N2O2	266.30
12222-75-2			Disperse Blue 35; CI 63265	CNc3c(c2c(cc3)C(=O)c1c(c(ccc1NC)O)C2=O)O	C16H14N2O4	298.30
3860-63-7	223-373-3		Disperse Blue 26; CI 63305	Oc3ccc(c2c3C(=O)c1c(c(ccc1NC)O)C2=O)NC	C16H14N2O4	298.30
103-41-3	203-109-3	GD 8400000	cinnamic acid, benzyl ester	O=C(OCc(cccc1)c1)C=Cc(cccc2)c2	C16H14O2	238.29
61-33-6		XH 9400000	Benzylopenicillin G	C3=CC=C(CC(=O)N[C@]2([H])C(=O)N1[C@]([H])(C(=O)O)C(S[C@]12[H])(C)C)C=C3	C16H18N2O4S	334.39
T-4735-007			3-geranyl catechol	c1ccc(O)c(O)c1C/C=C(/C)/CC/C=C(C)/C	C16H22O2	246.35
1120-48-5	214-311-6		di-n-octylamine	CCCCCCCCNCCCCCCCC	C16H35N	241.46
2475-46-9		CB 7350000	Disperse Blue 3; CI 61505; 9,10-anthraquinone, 1-NH-CH3, 4-NH-CH2CH2-OH	O=C(c(c(C(=O)c1c(NC)ccc2NCCO)c3)c3)c12	C17H16N2O3	296.33
126-07-8		WG 9800000	Griseofulvin	Clc1c(OC)cc(OC)c2C(=O)[C@@]3(Oc12)C(OC)=CC(=O)CC3C	C17H17ClO6	352.77
50-53-3		SN 8925000	chlorpromazine	c1cccc2sc3ccc(Cl)cc3N(c12)CCCN(C)C	C17H19ClN2S	318.86
T-4735-002			4-nitrosodiphenylamine	c1cc(N=O)ccc1N(c2cccc2)c3cccc3	C18H14N2O	274.32
7562-61-0		HP 5295050	D-(-)-usnic acid	C[C@@]12C3=C(OC1=CC(=O)C(=C2O)C(C)=O)C(=C(O)C(C)=C3O)C(C)=O	C18H16O7	344.32
3179-90-6		CB 0320000	Disperse Blue 7; CI 62500	O=C(c(c(c(NCCO)cc1)C(=O)c2c(O)cc3O)c1NCCO)c23	C18H18N2O6	358.35
53-86-1	200-186-5	NL 3500000	indomethacin; indometacin	COc1ccc2n(C(=O)c3ccc(Cl)cc3)c(C)c(CC(=O)O)c2c1	C19H16ClNO4	357.79
1166-52-5	214-620-6	DH 9100000	dodecyl gallate; lauryl gallate	O=C(OCCCCCCCCCCCC)c(cc(O)c(O)c1O)c1	C19H30O5	338.44

2944-28-7		Disperse Red 22	<chem>N(c1c3c(ccc1)C(=O)c2cccc2C3=O)c4cccc4</chem>	C20H13NO2	299.33	
12222-78-5	GD 0200000	Disperse Blue 73	<chem>Oc3ccc(cc3)c4c(c2c(c(c4)O)C(=O)c1c(ccc1N)O)C2=O)N</chem>	C20H14N2O5	362.34	
14233-37-5		Disperse Blue 134; Solvent Blue 36; CI 61551	<chem>CC(C)Nc3ccc(c2c3C(=O)c1c(cccc1)C2=O)NC(C)C</chem>	C20H22N2O2	322.41	
81-48-1	CB 7700000	Disperse Blue 72; CI 60725; Solvent Violet 13; D&C Violet 2	<chem>c1cccc2C(=O)c3c(Nc4ccc(C)cc4)ccc(O)c3C(=O)c12</chem>	C21H15NO3	329.35	
53237-59-5		urushiol; 3-pentadecadienyl catechol [position of double bonds not known]	<chem>c1ccc(O)c(O)c1CC=CC=CCCCCCC</chem>	C21H32O2	316.49	
15791-78-3	239-891-8	CB 6710000	Disperse Blue 27; 1,8-dihydroxy-4-nitro-5-(N-(p-phenethylalcohol)amino)-9,10-anthracenedione	<chem>Oc1ccc(Nc4ccc(CCO)cc4)c2c1C(=O)c(O)c(O)ccc3(N(=O)=O)c3C2(=O)</chem>	C22H16N2O7	420.38
81-68-5		Disperse Red 86	<chem>N(S(=O)(=O)c1ccc(C)cc1)C2=C4C(=C(N)C(=C2)OC)C(=O)c3cccc3C4=O</chem>	C22H18N2O5S	422.46	
83-89-6	AR 7700000	Atabrine; Quinacrine; acridine, 6-chloro-9-[[4-(diethylamino)-1-methylbutyl]amino]-2-methoxy-	<chem>CCN(CC)CCCC(C)Nc2c1ccc(Cl)cc1nc3ccc(OC)cc23</chem>	C23H30ClN3O	399.97	
51333-22-3	TU 3723000	Budesonide	<chem>[C@]12(C(=O)CO)[C@@]3(C)C[C@H](O)C4C5(C)C=CC(=O)C=C5CCC4[C@]3([H])C[C@H]1OC(CCC)O2</chem>	C25H34O6	430.54	
13609-67-1	GM 9002000	hydrocortisone, 17-butyrate	<chem>O=C1CC[C@]2(C)[C@@]3([H])[C@](O)([H])C[C@]4(C)[C@](C(=O)CO)(OC(=O)CCC)CC[C@]4([H])[C@]3([H])CCC2=C1</chem>	C25H36O6	432.56	
55560-96-8		tixocortol pivalate	<chem>C[C@]12CCC(=O)C=C1CC[C@]3([H])[C@@]2([H])[C@](O)([H])C[C@@]4(C)[C@@]3([H])CC[C@]4(O)C(=O)CSC(=O)C(C)(C)C</chem>	C26H38O5S	462.65	
1328-24-1		Acid Black 48; CI 65005	<chem>c1cccc2C(=O)c3c(N)ccc(c3C(=O)c12)Nc1ccc(N)c2C(=O)c3cccc3C(=O)c12</chem>	C28H17N3O4	459.46	
8006-99-3	FM 2997000	chenopodium oil; wormseed oil	unavailable	unavailable	unavailable	
T-1573-003		Disperse Blue 153	unavailable	unavailable	unavailable	
T-4735-006		Ludovicin-B	unavailable	unavailable	unavailable	

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