

Appendix D

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications

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Appendix D1

BCOP Data Sorted by Reference

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Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Alkyl phosphoric acid ester/amine salt	-	liquid	100%	n.p.	-	91.3	Severe	Severe	Category 1	4	SCNM	R41	Bailey et al. (2004)
Aromatic hydrocarbon #1	-	liquid	100%	n.p.	-	2.7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Aromatic hydrocarbon #2	-	liquid	100%	n.p.	-	4.6	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Aryl phosphonates	-	liquid	100%	n.p.	-	41.3	Moderate	Moderate	Category 2B		SCNM	SCNM	Bailey et al. (2004)
Carboxylic acid amides	-	solid	100%	n.p.	-	27.5	Moderate	Moderate	Category 1	4	Category I	R41	Bailey et al. (2004)
2-Chloro-2,4,4-trimethylpentane	-	liquid	100%	n.p.	-	4.1	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Clarified slurry oil	-	liquid	100%	n.p.	-	2.3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Cutting fluid (conc.) #1	-	liquid	100%	n.p.	-	3.5	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Cutting fluid (conc.) #2	-	liquid	100%	n.p.	-	4.9	Mild	Mild	Nonirritant		Category III	Nonirritant	Bailey et al. (2004)
Ethylhexyl acid phosphate ester	-	liquid	100%	n.p.	-	130.5	Severe	Severe	Category 1	4	SCNM	R41	Bailey et al. (2004)
5-Ethylidene-2-norbornene	16219-75-3	liquid	100%	n.p.	-	8.8	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Methyl cyclopentadiene dimer	-	liquid	100%	n.p.	-	0.7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Petroleum wax	-	solid	100%	n.p.	-	0.3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Polyalkenylsuccinate ester/amine salt	-	liquid	100%	n.p.	-	2.3	Mild	Mild	SCNM		Category III	SCNM	Bailey et al. (2004)
Process oil	-	liquid	100%	n.p.	-	2.7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Thiadiazole alkyl derivative	-	liquid	100%	n.p.	-	10.9	Moderate	Moderate	SCNM		Category III	SCNM	Bailey et al. (2004)
Acetone	67-64-1	liquid	100%	99	1	145.5	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Acetone	67-64-1	liquid	100%	99	2	119.5	Very severe						Balls et al. (1995)
Acetone	67-64-1	liquid	100%	99	3	120.4	Very severe						Balls et al. (1995)
Acetone	67-64-1	liquid	100%	99	4	131.72	Very severe						Balls et al. (1995)
Acetone	67-64-1	liquid	100%	99	5	98.4	Very severe						Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	1	8.3	Mild	Mild	Category 2B		Category III	R36	Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	2	6.4	Mild						Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	3	7.2	Mild						Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	4	21.82	Mild						Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	5	5.2	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	1	1.8	Mild	Mild	SCNM ¹¹		SCNM	SCNM	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	2	0.1	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	3	2.6	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	4	0.788	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	5	1.2	Mild						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	1	142.2	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	2	157.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	3	123.8	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	4	137.5	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	5	121.1	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	1	126.6	Very severe	Very Severe	Category 1	2	Category I	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	2	163.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	3	110.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	4	130.41	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	5	111.1	Very severe						Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	1	112.8	Very severe	Very Severe	Category 1	1	Category II	R41	Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	2	90.5	Very severe						Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	3	99.4	Very severe						Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	4	62.49	Severe						Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	5	78.6	Severe						Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	1	173	Very severe	Very Severe	Category 1	2	SCNM	R41	Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	2	288.7	Very severe						Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	3	91.1	Very severe						Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	4	149.86	Very severe						Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	5	145.3	Very severe						Balls et al. (1995)
Butyl acetate	123-86-4	liquid	100%	99	1	49.5	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Butyl acetate	123-86-4	liquid	100%	99	2	37.5	Moderate						Balls et al. (1995)
Butyl acetate	123-86-4	liquid	100%	99	3	43.9	Moderate						Balls et al. (1995)

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Butyl acetate	123-86-4	liquid	100%	99	4	23.86	Mild						Balls et al. (1995)
Butyl acetate	123-86-4	liquid	100%	99	5	18.1	Mild						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	1	90.6	Very severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	2	32.9	Moderate						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	3	31.5	Moderate						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	4	81.55	Very severe						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	5	67.1	Severe						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	1	27.8	Moderate	Moderate	Category 1	4	Category I	R41	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	2	27.2	Moderate						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	3	34.8	Moderate						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	4	102.918	Very severe						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	5	26.4	Moderate						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1	97.6	Very severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2	98.1	Very severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3	57.5	Severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	4	64.33	Severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	5	73.9	Severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	1	72.2	Severe	Severe	Category 1	2	SCNM	R41	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	2	86.3	Very severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	3	63.6	Severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	4	68.72	Severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	5	65.4	Severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	1	43.5	Moderate	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	2	89.6	Very severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	3	81	Very severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	4	71.22	Severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	5	76.7	Severe						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	1	11	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	2	4.1	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	3	12.1	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	4	4.33	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	5	14.5	Mild						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p. ¹²	1	147	Very severe	Very Severe	Category 1	4	SCNM	SCNM	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	2	122.9	Very severe						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	3	97.3	Very severe						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	4	101.78	Very severe						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	5	101.5	Very severe						Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	1	85	Very severe	Moderate	Category 1	2	Category I	R41	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	2	49.9	Moderate						Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	3	70.1	Severe						Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	4	52.24	Moderate						Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	5	43.2	Moderate						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	1	304.1	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	2	391.1	Very severe						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	3	418	Very severe						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	4	467.09	Very severe						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	5	307.5	Very severe						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	1	9.9	Mild	Mild	Category 2A		Category II	SCNM	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	2	11.2	Mild						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	3	10.8	Mild						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	4	14.43	Mild						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	5	5.6	Mild						Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	1	103.8	Very severe						Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	2	115	Very severe						Balls et al. (1995)

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2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	3	131.7	Very severe	Very Severe	SCNM		Category I	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	4	130.26	Very severe						Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	5	78.8	Severe	Mild	Category 1	1	Category I	R41	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	1	18.2	Mild						Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	2	25.3	Moderate	Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	3	20.5	Mild						Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	4	31.533	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	5	8.3	Mild						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	1	74.4	Severe	Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	2	53.2	Moderate						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	3	63.3	Severe	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	4	98.01	Very severe						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	5	64.2	Severe	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	1	19.7	Mild						Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	2	28.4	Moderate	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	3	47.1	Moderate						Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	4	44.31	Moderate	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	5	20.6	Mild						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	1	62	Severe	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	2	28.2	Moderate						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	3	30.7	Moderate	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	4	58.71	Severe						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	5	19.6	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	1	27.5	Moderate						Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	2	14.1	Mild	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	3	5.5	Mild						Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	4	5.543	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	5	19.6	Mild						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	1	27.4	Moderate	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	2	33.7	Moderate						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	3	10.5	Mild	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	4	8.633	Mild						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	5	9	Mild	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	1	45.5	Moderate						Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	2	151.9	Very severe	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	3	64.9	Severe						Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	4	23.023	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	5	18.2	Mild						Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	1	-2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	2	-0.2	Mild						Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	3	0.3	Mild	Severe/Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	4	3.08	Mild						Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	5	0.1	Mild	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	100%	98	1	71.5	Severe						Balls et al. (1995)
n-Hexanol	111-27-3	liquid	100%	98	2	83.6	Very severe	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	100%	98	3	63.2	Severe						Balls et al. (1995)
n-Hexanol	111-27-3	liquid	100%	98	4	48.19	Moderate	Severe/Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	100%	98	5	42.9	Moderate						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	1	116.8	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	2	133.9	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	3	103.4	Very severe	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	4	118.7	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	5	90.8	Very severe	Moderate			Category III	Nonirritant	Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	1	54.4	Moderate						Balls et al. (1995)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Isobutanol	78-83-1	liquid	100%	99.9	2	74	Severe	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	3	67.7	Severe						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	4	41.78	Moderate						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	5	42.2	Moderate						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	1	39.7	Moderate	Severe	Category 2A		Category III	SCNM	Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	2	59.5	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	3	72.3	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	4	78.5	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	5	39.3	Moderate						Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	1	67	Severe	Nonsevere	SCNM		Category III	SCNM	Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	2	16.9	Mild						Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	3	21	Mild						Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	4	63.76	Severe						Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	5	33.8	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	1	71.2	Severe	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	2	46.5	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	3	51.6	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	4	53.9	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	5	51.1	Moderate						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	1	16.3	Mild	Mild	Category 2A		Category II	R36	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	2	5.9	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	3	10.1	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	4	17.53	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	5	11	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	1	3.8	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	2	4.6	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	3	1.4	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	4	1.71	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	5	2.7	Mild						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	1	93	Very severe	Severe	Category 2A		Category III	R36	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	2	67.4	Severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	3	52.2	Moderate						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	4	78.71	Severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	5	60.8	Severe						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	1	8.8	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	2	20.1	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	3	10.3	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	4	13.25	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	5	10.3	Mild						Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	1	120.8	Very severe	Very Severe	Category 1	NC	Category I	SCNM	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	2	66.3	Severe						Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	3	42	Moderate						Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	4	88.73	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	5	72.5	Severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	1	136	Very severe	Very Severe	Category 1	1	Category I	R41	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	2	144.9	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	3	161	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	4	161.2	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	5	143	Very severe						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	1	43.4	Moderate	Moderate	Category 2B		Category II	R36	Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	2	78.9	Severe						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	3	39.8	Moderate						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	4	14.54	Mild						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	5	28	Moderate						Balls et al. (1995)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Parafluoraniiline	371-40-4	liquid	100%	99	1	29.5	Moderate	Moderate	SCNM		SCNM	SCNM	Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	100%	99	2	26.4	Moderate						Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	100%	99	3	40.8	Moderate						Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	100%	99	4	31.82	Moderate						Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	100%	99	5	23.5	Moderate						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	1	0.6	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	2	2.5	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	3	-1.3	Nonirritant						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	4	1.08	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	5	2.8	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	1	16.2	Mild	Mild	SCNM		SCNM	SCNM	Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	2	22.9	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	3	12	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	4	17.38	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	5	6.5	Mild						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	1	120.3	Very severe	Very Severe	Category 1	3	Category I	R41	Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	2	84.2	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	3	125.7	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	4	123.09	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	5	153.8	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	1	140.7	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	2	145.4	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	3	132.4	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	4	199.02	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	5	122.7	Very severe						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	1	0.3	Mild	Mild	Category 1	1	Category I	R41	Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	2	0.4	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	3	2.1	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	4	1.85	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	5	3.1	Mild						Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	1	285.2	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	2	224.1	Very severe						Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	3	254.7	Very severe						Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	4	348.27	Very severe						Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	5	247.2	Very severe						Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	1	167.4	Very severe	Very Severe	Category 2B		Category III	R36	Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	2	133.2	Very severe						Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	3	146.5	Very severe						Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	4	171.08	Very severe						Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	5	132.3	Very severe						Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	1	31.7	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	2	31.7	Moderate						Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	3	27.3	Moderate						Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	4	26.22	Moderate						Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	5	12.3	Mild						Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	1	47.3	Moderate	Severe	Category 1	NC	Category I	R36	Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	2	93	Very severe						Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	3	63.2	Severe						Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	4	59.61	Severe						Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	5	53.3	Moderate						Balls et al. (1995)
Sodium oxalate	62-76-0	solid	20%	>99	1	2.1	Mild	Mild	Category 1	4	Category I	R41	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	20%	>99	2	7.6	Mild						Balls et al. (1995)
Sodium oxalate	62-76-0	solid	20%	>99	3	5.8	Mild						Balls et al. (1995)
Sodium oxalate	62-76-0	solid	20%	>99	4	49.59	Moderate						Balls et al. (1995)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Sodium oxalate	62-76-0	solid	20%	>99	5	4.9	Mild	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	1	143.6	Very severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	2	118.4	Very severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	3	96.2	Very severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	4	64.531	Severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	5	62.9	Severe	Balls et al. (1995)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	1	23.6	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	2	7.9	Mild						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	3	14.2	Mild						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	4	20.65	Mild						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	5	8.9	Mild						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	1	149.4	Very severe	Very Severe	Animal died		Animal died	Animal died	Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	2	139.2	Very severe						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	3	135.6	Very severe						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	4	137.44	Very severe						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	5	99.1	Very severe						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	1	43.3	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	2	33.2	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	3	37.2	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	4	38.41	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	5	26.1	Moderate						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	1	272	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	2	225	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	3	296.9	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	4	323.08	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	5	203.7	Very severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	1	81.9	Very severe	Severe/Very Severe	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	2	49.8	Moderate						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	3	75.3	Severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	4	92.97	Very severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	5	79.3	Severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	1	74.3	Severe	Very Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	2	106.6	Very severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	3	80.2	Very severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	4	76.79	Very severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	5	53.6	Moderate						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	1	85.7	Very severe	Severe/Very Severe	Category 1	NC	Category II	R41	Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	2	76	Severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	3	86.1	Very severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	4	57.58	Severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	5	46.2	Moderate						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	1	-0.6	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	2	-1.1	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	3	-1.6	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	4	2.711	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	5	0.4	Mild						Balls et al. (1995)
Anti-Dandruff Shampoo (HZY)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Baby Shampoo No. 1 (HZZ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Baby Shampoo No. 2 (HZZ)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Bubble Bath (HZK)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)

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Cleansing Gel (HZQ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Eye Make-Up Remover (HZH)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Facial Cleanser (HZZ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Foam Bath (HZL)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Gel Cleanser (HZE)	-	n.p.	100%	n.p.	-	-	Mild	Mild	SCNM		Category I	SCNM	Casterton et al. (1996)
Mild Shampoo (HZJ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Polishing Scrub (HZT)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Shampoo No. 7 (HZA)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Shower Gel (HZS)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Skin Cleanser (HZI)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Acetone	67-64-1	liquid	100%	n.p.	-	-	Severe	Severe	Category 2A		Category II	R36	Casterton et al. (1996)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	n.p.	-	-	Severe	Severe	Category 1	1	Category I	R41	Casterton et al. (1996)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	n.p.	-	-	Severe	Severe	Category 1	2	Category I	R41	Casterton et al. (1996)
4-Bromophenotole	-	n.p.	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
n-Butanol	71-36-3	liquid	100%	n.p.	-	-	Severe	Severe					Casterton et al. (1996)
2-Butoxyethanol	111-76-2	liquid	100%	n.p.	-	-	Severe	Severe					Casterton et al. (1996)
4-Carboxybenzaldehyde	619-66-9	solid	100%	n.p.	-	-	Mild	Mild	Category 2A		Category II	R36	Casterton et al. (1996)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Cetylpyridinium bromide (1%)	140-72-7	liquid	1%	n.p.	-	-	Moderate	Moderate					Casterton et al. (1996)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	n.p.	-	-	Severe	Severe	Category 1	2	SCNM	R41	Casterton et al. (1996)
Cyclohexanol	108-93-0	liquid	100%	n.p.	-	-	Severe	Severe	Category 1	2	Category I	R41	Casterton et al. (1996)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	n.p.	-	-	Mild	Mild	Category 2A		Category II	SCNM	Casterton et al. (1996)
2,4-Difluoronitrobenzene	446-35-5	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
1,3-Diisopropylbenzene	99-62-7	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	n.p.	-	-	Severe	Severe	SCNM		Category I	SCNM	Casterton et al. (1996)
Dodecane	112-40-3	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
2-Ethylhexanol	104-76-7	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 2A		Category II	R36	Casterton et al. (1996)
3-Ethyltoluene	620-14-4	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	n.p.	-	-	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Glycerol	56-81-5	liquid	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
1,5-Hexadiene	592-42-7	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Isobutanol	78-83-1	liquid	100%	n.p.	-	-	Severe	Severe	Category 2A		Category II	R36	Casterton et al. (1996)
Isopropanol	67-63-0	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 2A		Category III	SCNM	Casterton et al. (1996)
Methyl acetate	79-20-9	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 2A		Category II	R36	Casterton et al. (1996)
Methyl ethyl ketone	78-93-3	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 2A		Category III	R36	Casterton et al. (1996)
Methyl isobutyl ketone	108-10-1	liquid	100%	n.p.	-	-	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
1-Methylpropyl benzene	135-98-8	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Paraffluoraniline	371-40-4	liquid	100%	n.p.	-	-	Moderate	Moderate	SCNM		SCNM	SCNM	Casterton et al. (1996)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Polyethylene glycol 600	-	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Propylene glycol	57-55-6	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	n.p.	-	-	Severe	Severe	Category 2B		Category III	R36	Casterton et al. (1996)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	n.p.	-	-	Moderate	Moderate	Category 1	NC	Category I	R36	Casterton et al. (1996)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Sodium lauryl sulfate (30 %)	151-21-3	liquid	30%	n.p.	-	-	Moderate	Moderate					Casterton et al. (1996)
Toluene	108-88-3	liquid	100%	n.p.	-	-	Severe	Severe	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Triton X-100 (5%)	9002-93-1	liquid	5%	n.p.	-	-	Moderate	Moderate	Category 2A		Category III	Nonirritant	Casterton et al. (1996)
Triton X-100 (1%)	9002-93-1	liquid	1%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Triton X-100 (10%)	9002-93-1	liquid	100%	n.p.	-	-	Severe	Severe	Category 1	NC	Category II	R41	Casterton et al. (1996)
Tween 20	9005-64-5	liquid	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Xylene	1330-20-7	liquid	100%	n.p.	-	-	Moderate	Moderate	Nonirritant		Category II	Nonirritant	Casterton et al. (1996)
Amway all fabric bleach	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway automatic dishwashing compound for soft water	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway automatic dishwashing compound, standard formula	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway concrete floor cleaner	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	SCNM	R41	Casterton et al. (1996)
Amway Dish Drops dishwashing liquid	-	n.p.	100%	n.p.	-	-	Moderate	Moderate					Casterton et al. (1996)
Amway dry chlorine bleach	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway fabric softener	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Amway Kool Wash delicate fabric detergent	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R36	Casterton et al. (1996)
Amway LOC all purpose cleaner	-	n.p.	100%	n.p.	-	-	Mild	Mild	SCNM		SCNM	Nonirritant	Casterton et al. (1996)
Amway prewash liquid	-	liquid	100%	n.p.	-	-	Mild	Mild	SCNM		Category I	SCNM	Casterton et al. (1996)
Amway Pursue disinfectant cleaner	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway Redu dye stain remover	-	n.p.	100%	n.p.	-	-	Mild	Mild	Category 2A		Category II	Nonirritant	Casterton et al. (1996)
Amway SA8 laundry liquid	-	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Amway SA8 limited phos laundry powder	-	solid	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Allyl alcohol	107-18-6	liquid	100%	n.p.	1	156	Severe	Severe	Category 2A		Category III	R36	Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	2	138	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	3	232	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	4	156	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	5	132	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	6	191	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	7	190	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	8	166	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	9	123	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	10	101	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	11	200	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	12	90	Severe						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	1	5	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	2	4	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	3	10	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	4	3	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	5	5	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	6	28	Moderate						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	7	2	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	8	4	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	9	10	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	10	6	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	11	2	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	12	2	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	1	7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	2	5	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	3	3	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	4	5	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	5	6	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	6	7	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	7	5	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	8	6	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	9	13	Mild						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
2-Aminophenol	95-55-6	solid	20%	n.p.	10	11	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	11	5	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	12	11	Mild						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	1	-2	Nonirritant						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	3	-3	Nonirritant						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	4	0	Mild						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	6	-1	Nonirritant						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	7	0	Mild						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	8	0	Mild						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	10	0	Mild						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	12	2	Mild	Gautheron et al. (1994)										
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	1	128	Severe	Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	2	124	Severe						Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	3	163	Severe						Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	4	106	Severe						Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	5	128	Severe						Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	6	129	Severe						Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	7	142	Severe						Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	8	129	Severe						Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	9	166	Severe						Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	10	no data	n.a. ¹³						Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	11	142	Severe						Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	12	116	Severe						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	1	4	Mild						Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	2	1	Mild											Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	3	0	Mild	Gautheron et al. (1994)										
Betaine monohydrate	590-47-6	solid	20%	n.p.	4	1	Mild	Gautheron et al. (1994)										
Betaine monohydrate	590-47-6	solid	20%	n.p.	5	1	Mild	Gautheron et al. (1994)										
Betaine monohydrate	590-47-6	solid	20%	n.p.	6	3	Mild	Gautheron et al. (1994)										
Betaine monohydrate	590-47-6	solid	20%	n.p.	7	1	Mild	Gautheron et al. (1994)										
Betaine monohydrate	590-47-6	solid	20%	n.p.	8	-10	Nonirritant	Gautheron et al. (1994)										
Betaine monohydrate	590-47-6	solid	20%	n.p.	9	4	Mild	Gautheron et al. (1994)										
Betaine monohydrate	590-47-6	solid	20%	n.p.	10	-1	Nonirritant	Gautheron et al. (1994)										
Betaine monohydrate	590-47-6	solid	20%	n.p.	11	1	Mild	Gautheron et al. (1994)										
Betaine monohydrate	590-47-6	solid	20%	n.p.	12	6	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	1	0	Mild	Mild	Nonirritant		Category IV	Nonirritant						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	2	2	Mild											Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	3	-1	Nonirritant						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	4	1	Mild						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	5	0	Mild						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	6	0	Mild						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	7	0	Mild						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	8	0	Mild						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	9	1	Mild						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	12	-2	Nonirritant						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	1	48	Moderate										Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	100%	n.p.	2	44	Moderate										Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	100%	n.p.	3	64	Severe	Gautheron et al. (1994)										

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Butyrolactone	96-48-0	liquid	100%	n.p.	4	35	Moderate	Moderate	Category 2A		Category II	R36	Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	5	35	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	6	30	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	7	80	Severe						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	8	32	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	9	42	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	10	53	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	11	35	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	12	49	Moderate						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	1	92	Severe						Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	100%	n.p.	2	108	Severe											Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	100%	n.p.	3	96	Severe											Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	100%	n.p.	4	81	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	5	130	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	6	93	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	7	104	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	8	90	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	9	142	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	11	118	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	12	108	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	1	96	Severe	Severe	Category 2A		Category II	R36	Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	2	72	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	3	106	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	4	73	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	5	119	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	6	103	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	7	88	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	8	46	Moderate						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	9	100	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	10	60	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	11	200	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	12	59	Severe						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	1	53	Moderate	Moderate	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	2	41	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	3	105	Severe						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	4	39	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	5	42	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	6	34	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	7	49	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	8	41	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	9	92	Severe						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	11	36	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	12	56	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	1	104	Severe	Severe	Category 1	2	Category I	R41	Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	2	134	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	3	82	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	4	118	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	5	110	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	6	66	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	7	88	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	8	193	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	9	82	Severe						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	10	no data	n.a.	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	11	213	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	12	135	Severe						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	1	23	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	2	23	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	3	18	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	4	28	Moderate						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	5	16	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	6	31	Moderate						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	7	18	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	8	71	Severe						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	9	19	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	10	20	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	11	34	Moderate						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	12	14	Mild						Gautheron et al. (1994)					
Dimethylbiguanide	657-24-9	solid	20%	n.p.	1	0	Mild						Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	2	3	Mild											Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	3	1	Mild											Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	4	3	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	5	1	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	6	5	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	7	3	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	8	1	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	9	2	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	11	5	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	12	8	Mild	Gautheron et al. (1994)										
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	1	10	Mild	Mild	Nonirritant		Category III	Nonirritant						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	2	10	Mild											Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	3	14	Mild											Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	4	11	Mild											Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	5	11	Mild											Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	6	14	Mild											Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	7	10	Mild						Gautheron et al. (1994)					
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	8	10	Mild						Gautheron et al. (1994)					
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	9	9	Mild						Gautheron et al. (1994)					
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	11	4	Mild						Gautheron et al. (1994)					
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	12	22	Mild						Gautheron et al. (1994)					
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	1	-1	Mild						Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	2	0	Mild											Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	3	-8	Mild											Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	4	2	Mild											Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	5	2	Mild											Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	6	2	Mild											Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	7	1	Mild	Gautheron et al. (1994)										
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	8	-6	Mild	Gautheron et al. (1994)										
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	9	1	Mild	Gautheron et al. (1994)										
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	10	-1	Mild	Gautheron et al. (1994)										
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	11	3	Mild	Gautheron et al. (1994)										
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	12	1	Mild	Gautheron et al. (1994)										
Ethanol	64-17-5	liquid	100%	n.p.	1	58	Severe											Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	2	67	Severe											Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	3	70	Severe											Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Ethanol	64-17-5	liquid	100%	n.p.	4	45	Moderate	Severe	SCNM		Category II	Nonirritant	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	5	60	Severe						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	6	64	Severe						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	7	58	Severe						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	8	51	Moderate						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	9	46	Moderate						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	11	104	Severe						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	12	45	Moderate						Gautheron et al. (1994)					
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	1	99	Severe						Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	2	100	Severe											Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	3	128	Severe											Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	4	75	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	5	75	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	6	85	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	7	94	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	8	93	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	9	84	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	10	75	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	11	101	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	12	86	Severe	Gautheron et al. (1994)										
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	1	26	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	2	38	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	3	31	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	4	33	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	5	21	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	6	29	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	7	28	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	8	38	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	9	26	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	11	38	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	12	42	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	1	73	Severe	Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	2	63	Severe						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	3	61	Severe						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	4	65	Severe						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	5	33	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	6	34	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	7	87	Severe						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	8	48	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	9	50	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	10	39	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	11	68	Severe						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	12	51	Moderate						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	1	63	Severe	Severe	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	2	81	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	3	90	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	4	62	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	5	108	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	6	66	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	7	90	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	8	57	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	9	88	Severe						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Gluconolactone	90-80-2	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	11	75	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	12	63	Severe						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	1	2	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	3	1	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	4	1	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	6	-4	Nonirritant	Mild	SCNM		SCNM	SCNM	Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	8	4	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	9	0	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	10	2	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	11	0	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	12	-1	Nonirritant						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	1	18	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	2	24	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	3	25	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	4	14	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	5	13	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	6	6	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	7	15	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	8	18	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	9	18	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	10	4	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	11	23	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	12	21	Mild						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1	93	Severe						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2	40	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3	53	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	4	33	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	5	91	Severe						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	6	42	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	7	82	Severe	Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	8	76	Severe						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	9	70	Severe						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	11	48	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	12	102	Severe						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	1	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	2	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	3	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	4	0	Mild						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Hexane	110-54-3	liquid	100%	n.p.	5	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	6	1	Mild						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	7	3	Mild						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	8	1	Mild						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	9	1	Mild						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	10	-1	Nonirritant						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	12	6	Mild						Gautheron et al. (1994)					
Imidazole	288-32-4	solid	20%	n.p.	1	75	Severe						Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	2	73	Severe											Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	3	140	Severe											Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	4	81	Severe											Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	5	96	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	6	62	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	7	82	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	8	122	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	9	64	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	10	81	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	11	114	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	12	65	Severe	Gautheron et al. (1994)										
Iminodibenzyl	494-19-9	solid	20%	n.p.	1	0	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	3	6	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	4	0	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	5	4	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	6	0	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	8	12	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	9	0	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	10	no data	n.a						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	11	6	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	12	-4	Nonirritant						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	1	53	Moderate	Moderate	Category 2B		Category III	Nonirritant	Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	2	50	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	3	48	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	4	28	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	5	45	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	6	35	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	7	48	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	8	43	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	9	63	Severe						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	10	no data	n.a						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	11	89	Severe						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	12	48	Moderate						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	1	81	Severe	Severe	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	2	82	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	3	103	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	4	76	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	5	92	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	6	68	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	7	90	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	8	62	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	9	102	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	10	no data	n.a						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	11	76	Severe	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	12	55	Moderate						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	1	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	2	6	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	3	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	4	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	6	1	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	7	7	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	8	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	11	0	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	1	0	Mild						Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	2	-1	Nonirritant											Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	3	-1	Nonirritant											Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	4	1	Mild											Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	5	0	Mild	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	6	1	Mild	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	7	0	Mild	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	8	-8	Nonirritant	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	9	0	Mild	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	10	0	Mild	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	11	-4	Nonirritant	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	12	-3	Nonirritant	Gautheron et al. (1994)										
Methanol	67-56-1	liquid	100%	n.p.	1	88	Severe	Severe	Nonirritant		Category II	Nonirritant	Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	2	88	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	3	54	Moderate						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	4	71	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	5	81	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	6	108	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	7	37	Moderate						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	8	19	Mild						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	9	99	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	11	179	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	12	102	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	1	61	Severe	Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	2	69	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	3	66	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	4	47	Moderate						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	5	48	Moderate						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	6	62	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	7	65	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	8	62	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	9	57	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	11	74	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	12	88	Severe						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	1	22	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	2	25	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	3	27	Moderate						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	4	19	Mild						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	5	21	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	6	23	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	7	16	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	8	16	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	9	19	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	11	20	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	12	11	Mild						Gautheron et al. (1994)					
MYRJ-45	-	surfactant	10%	n.p.	1	2	Mild						Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	2	1	Mild											Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	3	0	Mild											Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	4	1	Mild											Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	5	0	Mild	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	6	0	Mild	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	7	1	Mild	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	8	-4	Nonirritant	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	9	1	Mild	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	11	-3	Nonirritant	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	12	-1	Nonirritant	Gautheron et al. (1994)										
1-Nitropropane	108-03-2	liquid	100%	n.p.	1	11	Mild	Mild	Nonirritant		Category IV	Nonirritant						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	2	8	Mild											Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	3	9	Mild											Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	4	4	Mild											Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	5	6	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	6	7	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	7	6	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	8	6	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	9	17	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	10	4	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	11	6	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	12	7	Mild						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	1	65	Severe						Moderate	Category 2B		Category III	R36	Gautheron et al. (1994)
Octanol	111-87-5	liquid	100%	n.p.	2	33	Moderate											Gautheron et al. (1994)
Octanol	111-87-5	liquid	100%	n.p.	3	42	Moderate	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	4	49	Moderate	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	5	66	Severe	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	6	48	Moderate	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	7	37	Moderate	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	8	25	Mild	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	9	61	Severe	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	11	31	Moderate	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	12	64	Severe	Gautheron et al. (1994)										
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	1	61	Severe	Severe	Nonirritant		Category III	Nonirritant						Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	2	79	Severe											Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	3	75	Severe						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	4	34	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	5	70	Severe						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	6	46	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	7	54	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	8	44	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	9	50	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	10	67	Severe						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	11	62	Severe	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	12	76	Severe						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	1	8	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	2	13	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	3	11	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	4	1	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	5	2	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	6	5	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	7	7	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	8	0	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	9	2	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	10	3	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	11	5	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	12	9	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	1	0	Mild						Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	2	1	Mild											Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	3	1	Mild											Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	4	0	Mild											Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	5	0	Mild	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	6	1	Mild	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	7	0	Mild	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	8	-6	Nonirritant	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	9	1	Mild	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	10	1	Mild	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	11	-3	Nonirritant	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	12	2	Mild	Gautheron et al. (1994)										
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	1	7	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	2	12	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	3	15	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	4	9	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	5	28	Moderate						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	6	6	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	7	6	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	8	16	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	9	13	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	10	15	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	11	13	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	12	15	Mild						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	1	117	Severe	Severe	Category 1	3	Category I	R41	Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	2	156	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	3	109	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	4	111	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	5	164	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	6	174	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	7	103	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	8	50	Moderate						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	9	139	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	11	94	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	12	19	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	1	7	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	2	7	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	3	14	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	4	4	Mild						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	5	6	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	6	9	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	7	6	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	8	11	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	9	6	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	11	12	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	12	5	Mild						Gautheron et al. (1994)					
Pyridine	110-86-1	liquid	100%	n.p.	1	102	Severe						Severe	Category 1	4	Category II	R41	Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	2	123	Severe											Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	3	186	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	4	79	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	5	102	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	6	77	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	7	124	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	8	132	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	9	105	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	11	96	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	12	115	Severe	Gautheron et al. (1994)										
Quinacrine	69-05-6	solid	20%	n.p.	1	17	Mild	Moderate	Category 1	1	Category I	R41						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	2	29	Moderate											Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	3	8	Mild						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	4	46	Moderate						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	5	52	Moderate						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	6	24	Mild						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	7	15	Moderate						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	8	18	Moderate						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	9	58	Severe						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	11	3	Mild						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	12	72	Severe						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	1	2	Mild						Mild	Category 1	4	Category I	R41	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	2	2	Mild											Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	3	9	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	4	5	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	5	3	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	6	2	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	7	4	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	8	3	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	9	3	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	10	9	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	11	11	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	12	4	Mild	Gautheron et al. (1994)										
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	1	5	Mild	Mild	Nonirritant		Category II	Nonirritant						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	2	1	Mild											Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	3	2	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	4	6	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	6	4	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	7	2	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	8	19	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	9	3	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	11	18	Mild	Severe	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	1	146	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	2	175	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	3	169	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	4	152	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	5	140	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	6	120	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	7	129	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	8	173	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	9	151	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	11	203	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	12	104	Severe						Gautheron et al. (1994)					
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	1	47	Moderate						Moderate	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	2	42	Moderate											Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	3	78	Severe	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	4	28	Moderate	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	5	42	Moderate	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	6	47	Moderate	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	7	48	Moderate	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	8	24	Mild	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	9	91	Severe	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	11	28	Moderate	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	12	47	Moderate	Gautheron et al. (1994)										
Triethanolamine	102-71-6	liquid	100%	n.p.	1	2	Mild	Mild			Category IV	Nonirritant	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	2	4	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	3	0	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	4	0	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	5	-1	Nonirritant						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	6	1	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	7	1	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	8	3	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	9	3	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	11	5	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	12	6	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	1	25	Mild	Mild			Category III	Nonirritant	Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	2	14	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	3	26	Moderate						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	4	11	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	5	27	Moderate						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	6	7	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	7	9	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	8	15	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	9	21	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	10	10	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	11	7	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	12	21	Mild						Gautheron et al. (1994)					
Triton X-155	9010-44-0	surfactant	10%	n.p.	1	-1	Nonirritant						Gautheron et al. (1994)					
Triton X-155	9010-44-0	surfactant	10%	n.p.	2	1	Mild						Gautheron et al. (1994)					
Triton X-155	9010-44-0	surfactant	10%	n.p.	3	-1	Nonirritant						Gautheron et al. (1994)					
Triton X-155	9010-44-0	surfactant	10%	n.p.	4	0	Mild						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Triton X-155	9010-44-0	surfactant	10%	n.p.	5	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	6	2	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	7	0	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	8	2	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	9	3	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	12	0	Mild						Gautheron et al. (1994)
Anti-Dandruff Shampoo (HZY) 100%	-	n.p.	10%	n.p.	-	20.8	Severe	Severe	Category I	1	Category I	R41	Gettings et al. (1996)
Babv Shampoo No. 1 (HZP) 100%	-	n.p.	10%	n.p.	-	4.0	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Babv Shampoo No. 2 (HZF) 100%	-	n.p.	10%	n.p.	-	8.3	Nonsevere	Nonsevere	Category 1	1	Category I	R41	Gettings et al. (1996)
Bubble Bath (HZK) 100%	-	n.p.	10%	n.p.	-	17.5	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Cleansing Gel (HZQ) 100%	-	n.p.	10%	n.p.	-	2.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Eye Make-Up Remover (HZH) 100%	-	n.p.	10%	n.p.	-	0.2	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Facial Cleansing Foam (HZR) 25%	-	n.p.	10%	n.p.	-	4.1	Nonsevere	Nonsevere	SCNM		Category I	SCNM	Gettings et al. (1996)
Facial Cleanser (HZZ) 100%	-	n.p.	10%	n.p.	-	1.8	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Foam Bath (HZL) 100%	-	n.p.	10%	n.p.	-	18.6	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Gel Cleanser (HZE) 100%	-	n.p.	10%	n.p.	-	3.1	Nonsevere	Nonsevere	SCNM		Category I	SCNM	Gettings et al. (1996)
Hand Soap (HZU) 25%	-	n.p.	10%	n.p.	-	5.5	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Liquid Soap No. 2 (HZW) 25%	-	n.p.	10%	n.p.	-	5.6	Nonsevere	Nonsevere	Category 2B		Category III	Nonirritant	Gettings et al. (1996)
Liquid Soap No. 1 (HZB) 25%	-	n.p.	10%	n.p.	-	2.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Mild Shampoo (HZJ) 25%	-	n.p.	10%	n.p.	-	0.1	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Polishing Scrub (HZZ) 100%	-	n.p.	10%	n.p.	-	3.7	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Shampoo No. 1 (HZC) 25%	-	n.p.	10%	n.p.	-	30.0	Severe	Severe	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 2 (HZZ)	-	n.p.	10%	n.p.	-	14.0	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Shampoo No. 3 (HZM) 25%	-	n.p.	10%	n.p.	-	4.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 4 (HZV) 25%	-	n.p.	10%	n.p.	-	8.4	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 5 (HZD) 25%	-	n.p.	10%	n.p.	-	2.7	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 6 (HZN) 25%	-	n.p.	10%	n.p.	-	4.5	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 7 (HZA) 100%	-	n.p.	10%	n.p.	-	6.6	Nonsevere	Nonsevere	Category 1	1	Category I	R41	Gettings et al. (1996)
Shampoo No. 8 (HZG) 25%	-	n.p.	10%	n.p.	-	2.7	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shower Gel (HZS) 100%	-	n.p.	10%	n.p.	-	35.9	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Skin Cleanser (HZI) 100%	-	n.p.	10%	n.p.	-	15.8	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	1 (1)	4.9	Mild	Mild	Category 2B		Category III	R36	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	1 (2)	5.9	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	2 (1)	3.9	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	2 (2)	3.6	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	3 (1)	5.2	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	3 (2)	6.7	Mild						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (1)	195.2	Very severe	Very Severe	Category 1	4	SCNM	R41	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (2)	135.2	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (3)	137.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (4)	156.5	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (5)	138.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (6)	176.8	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (7)	183.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (8)	175.4	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (1)	154.4	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (2)	156.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (3)	150.8	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (4)	157.2	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (5)	157.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (6)	157.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (7)	160.2	Very severe						Southee (1998)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (1)	156.9	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (2)	163.4	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (3)	169.7	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (4)	162.8	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (5)	151.6	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (6)	163.1	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (7)	167.8	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (8)	156.9	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (9)	160.0	Very severe						Southee (1998)					
Butyl cellulose	111-76-2	liquid	100%	n.p.	1 (1)	108.3	Very severe						Very Severe	Category 1	1	Category II	R41	Southee (1998)
Butyl cellulose	111-76-2	liquid	100%	n.p.	1 (2)	111.8	Very severe	Southee (1998)										
Butyl cellulose	111-76-2	liquid	100%	n.p.	2 (1)	92.8	Very severe	Southee (1998)										
Butyl cellulose	111-76-2	liquid	100%	n.p.	2 (2)	99.2	Very severe	Southee (1998)										
Butyl cellulose	111-76-2	liquid	100%	n.p.	3 (1)	94.9	Very severe	Moderate	Category 2A		Category II	R36	Southee (1998)					
Butyl cellulose	111-76-2	liquid	100%	n.p.	3 (2)	98.2	Very severe						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1 (1)	53.9	Moderate						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1 (2)	47.7	Moderate						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2 (1)	47.1	Moderate						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2 (2)	47.2	Moderate						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3 (1)	42.2	Moderate						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3 (2)	41.8	Moderate						Southee (1998)					
Ethanol	64-17-5	liquid	100%	n.p.	1 (1)	36.6	Moderate						Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (2)	37.6	Moderate											Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (3)	29.6	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	1 (4)	41.7	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	1 (5)	31.5	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	1 (6)	42.6	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	1 (7)	55.4	Severe	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (1)	52.7	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (2)	54.5	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (3)	61.7	Severe	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (4)	60.2	Severe	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (5)	54.2	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (6)	73.4	Severe	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (7)	64.0	Severe	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (8)	51.4	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (1)	47.0	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (2)	45.4	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (3)	44.4	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (4)	45.7	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (5)	54.6	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (6)	44.8	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (7)	42.2	Moderate	Southee (1998)										
Glycerol	56-81-5	liquid	100%	>99.5	1 (1)	0.6	Mild	Nonirritant	Nonirritant		Category IV	Nonirritant						Southee (1998)
Glycerol	56-81-5	liquid	100%	>99.5	1 (2)	0.3	Mild											Southee (1998)
Glycerol	56-81-5	liquid	100%	>99.5	2 (1)	0.8	Nonirritant											Southee (1998)
Glycerol	56-81-5	liquid	100%	>99.5	2 (2)	0.8	Nonirritant											Southee (1998)
Glycerol	56-81-5	liquid	100%	>99.5	3 (1)	1.0	Nonirritant											Southee (1998)
Glycerol	56-81-5	liquid	100%	>99.5	3 (2)	0.8	Nonirritant											Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1 (1)	23.1	Mild						Southee (1998)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1 (2)	17.2	Mild						Southee (1998)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2 (1)	34.6	Moderate	Moderate	Category 1	4	Category I	R41	Southee (1998)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2 (2)	39.1	Moderate						Southee (1998)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3 (1)	31.7	Moderate						Southee (1998)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3 (2)	29.9	Moderate						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (1)	142.0	Very severe	Very Severe	Category 1	4	Category I	R41	Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (2)	137.6	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (3)	112.2	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (4)	131.1	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (5)	145.6	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (6)	162.6	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (7)	125.5	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (1)	138.1	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (2)	140.1	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (3)	134.9	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (4)	157.2	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (5)	137.6	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (6)	152.9	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (7)	148.7	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (1)	139.6	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (2)	140.1	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (3)	124.0	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (4)	128.7	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (5)	123.4	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (6)	121.2	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (7)	131.3	Very severe	Southee (1998)										
Methyl ethyl ketone	78-93-3	liquid	100%	99	1 (1)	73.3	Severe	Severe	Category 2B		Category III	R36	Southee (1998)					
Methyl ethyl ketone	78-93-3	liquid	100%	99	1 (2)	67.8	Severe						Southee (1998)					
Methyl ethyl ketone	78-93-3	liquid	100%	99	2 (1)	108.7	Very severe						Southee (1998)					
Methyl ethyl ketone	78-93-3	liquid	100%	99	2 (2)	101.7	Very severe						Southee (1998)					
Methyl ethyl ketone	78-93-3	liquid	100%	99	3 (1)	70.2	Severe						Southee (1998)					
Methyl ethyl ketone	78-93-3	liquid	100%	99	3 (2)	73.5	Severe						Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	1 (1)	31	Moderate	Moderate	SCNM		SCNM	SCNM	Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	1 (2)	35	Moderate						Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	2 (1)	38.3	Moderate						Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	2 (2)	37.5	Moderate						Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	3 (1)	22.1	Mild						Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	3 (2)	28.9	Moderate						Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	1 (1)	11.2	Mild	Mild	Nonirritant		Category III	Nonirritant	Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	1 (2)	7.4	Mild						Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	2 (1)	5.2	Mild						Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	2 (2)	3.6	Mild						Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	3 (1)	7.7	Mild						Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	3 (2)	6.2	Mild						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	1 (1)	245.0	Very severe	Very Severe	Category 1	4	Category I	R41	Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	1 (2)	227.1	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	2 (1)	241.3	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	2 (2)	235.5	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	3 (1)	193.1	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	3 (2)	214.9	Very severe						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	1 (1)	5.4	Mild											Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	1 (2)	5.2	Mild											Southee (1998)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	2 (1)	15.9	Mild	Mild	Category 1	NC	Category I	SCNM	Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	2 (2)	17.3	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	3 (1)	8.7	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	3 (2)	5.6	Mild						Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	1 (1)	10.3	Mild	Nonirritant	Category 1	4	Category I	R41	Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	1 (2)	4.4	Mild						Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	2 (1)	-0.3	Nonirritant						Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	2 (2)	-0.1	Nonirritant						Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	3 (1)	2.7	Nonirritant						Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	3 (2)	4.5	Mild						Southee (1998)					
Triton X-100 (5%)	9002-93-1	liquid	10%	98	1 (1)	3.7	Mild						Mild	Category 2B		Category III	R36	Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	1 (2)	1.8	Mild											Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	2 (1)	5.8	Mild	Southee (1998)										
Triton X-100 (5%)	9002-93-1	liquid	10%	98	2 (2)	3.4	Mild	Southee (1998)										
Triton X-100 (5%)	9002-93-1	liquid	10%	98	3 (1)	3.0	Nonirritant	Southee (1998)										
Triton X-100 (5%)	9002-93-1	liquid	10%	98	3 (2)	1.9	Nonirritant	Southee (1998)										
Tween 20	9005-64-5	liquid	100%	98	1 (1)	0.3	Mild	Nonirritant	Nonirritant		Category III	Nonirritant	Southee (1998)					
Tween 20	9005-64-5	liquid	100%	98	1 (2)	0.0	Mild						Southee (1998)					
Tween 20	9005-64-5	liquid	100%	98	2 (1)	0.4	Mild						Southee (1998)					
Tween 20	9005-64-5	liquid	100%	98	2 (2)	0.4	Nonirritant						Southee (1998)					
Tween 20	9005-64-5	liquid	100%	98	3 (1)	0.3	Nonirritant						Southee (1998)					
Tween 20	9005-64-5	liquid	100%	98	3 (2)	0.0	Nonirritant						Southee (1998)					
1-1 (#1)	-	liquid	100%	n.p.	-	83.6	Severe	Severe	Category 2A		Category I	R36	Swanson and Harbell (2000)					
1-2 (#2)	-	liquid	100%	n.p.	-	12.4	Mild	Mild	Category 2A		Category II	R36	Swanson and Harbell (2000)					
1-3 (#3)	-	liquid	100%	n.p.	-	29.6	Moderate	Moderate	Category 2A		Category II	R36	Swanson and Harbell (2000)					
2-4 (#4)	-	liquid	100%	n.p.	-	7.3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Swanson and Harbell (2000)					
2-7 (#7)	-	liquid	100%	n.p.	-	21.4	Moderate	Moderate	Nonirritant		Category IV	Nonirritant	Swanson and Harbell (2000)					
2-8 (#8)	-	liquid	100%	n.p.	-	31.8	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Swanson and Harbell (2000)					
Benchmark-Group 1 (#12)	-	liquid	100%	n.p.	-	60.1	Severe	Severe	Category 2A		Category I	R36	Swanson and Harbell (2000)					
Benchmark-Group 2 (#13)	-	liquid	100%	n.p.	-	60.1	Severe	Severe	Category 1	1	Category I	R41	Swanson and Harbell (2000)					
Ethanol (#14)	64-17-5	liquid	100%	n.p.	-	52.7	Moderate	Moderate	Category 2A		Category I	R36	Swanson and Harbell (2000)					
Toilet Bowl Cleaner (#1)	-	liquid	100%	n.p.	-	13.5	Mild	Mild	Nonirritant		Category IV	Nonirritant	Swanson et al. (1995)					
Toilet Bowl Cleaner (#4)	-	liquid	100%	n.p.	-	15	Mild	Mild	Nonirritant		SCNM	Nonirritant	Swanson et al. (1995)					
All Purpose Cleaner (#5)	-	liquid	100%	n.p.	-	121.3	Severe	Severe					Swanson et al. (1995)					
Bathroom Cleaner (#6)	-	liquid	100%	n.p.	-	78.3	Severe	Severe	SCNM		Category III	Nonirritant	Swanson et al. (1995)					
All Purpose Cleaner (#7)	-	liquid	100%	n.p.	-	393.3	Severe	Severe					Swanson et al. (1995)					
Pot and Pan Cleaner (#8)	-	liquid	100%	n.p.	-	-0.6	Nonirritant	Nonirritant					Swanson et al. (1995)					
Heavy Duty Cleaner/Degreaser (#9)	-	liquid	100%	n.p.	-	354.7	Severe	Severe					Swanson et al. (1995)					
Floor Cleaner (#10)	-	liquid	100%	n.p.	-	70.3	Severe	Severe					Swanson et al. (1995)					
General Cleaner (#11)	-	liquid	100%	n.p.	-	83.3	Severe	Severe					Swanson et al. (1995)					
General Cleaner (#12)	-	liquid	100%	n.p.	-	113.5	Severe	Severe					Swanson et al. (1995)					
Cleaner/Degreaser (#13)	-	liquid	100%	n.p.	-	353.6	Severe	Severe					Swanson et al. (1995)					
Floor Stripper (#14)	-	liquid	100%	n.p.	-	157.3	Severe	Severe					Swanson et al. (1995)					
Heavy Duty Cleaner (#15)	-	liquid	100%	n.p.	-	357.1	Severe	Severe	Category 1	NC	Category I	R41	Swanson et al. (1995)					
Degreaser (#16)	-	liquid	100%	n.p.	-	255.7	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)					
Floor Stripper (#17)	-	liquid	100%	n.p.	-	216.2	Severe	Severe	Category 1	NC	Category I	R41	Swanson et al. (1995)					
Floor Stripper (#18)	-	liquid	100%	n.p.	-	444.3	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Glass Cleaner (#19)	-	liquid	100%	n.p.	-	135.8	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Metal Cleaner (#20)	-	liquid	100%	n.p.	-	391.9	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Floor Cleaner (#2)	-	liquid	100%	n.p.	-	-0.3	Nonirritant	Nonirritant					Swanson et al. (1995)
Meat Room Degreaser (#3)	-	liquid	100%	n.p.	-	140.3	Severe	Severe					Swanson et al. (1995)

¹CASRN=Chemical Abstract Services Registry Number

²*In Vitro* Classification represents the BCOP ocular irritancy classification assigned for each chemical in the study for each test for a specific substance

³Consensus classification represents the overall BCOP ocular irritancy classification assigned for each chemical in the study based on the majority of ocular irritancy classification calls

⁴GHS=Globally Harmonized System (UN [2003])

⁵Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye

⁶NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are both severe and persistent; and 4: corneal opacity score equal to 4 at any time; NC: not classified because none of the above criteria were met

⁷EPA=U.S. Environmental Protection Agency (EPA [1996]).

⁸Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 1-7 days; Category IV: minimal effects clearing in less than 24 hr

⁹EU=European Union (EU [2001]).

¹⁰Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

¹¹SCNM=Study Criteria Not Met

¹²n.p.=Not provided

¹³n.a.=Not applicable

Appendix D2

BCOP Data Sorted by Substance Name

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Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
1-1 (#1)	-	liquid	100%	n.p.	-	83.6	Severe	Severe	Category 2A		Category I	R36	Swanson and Harbell (2000)					
1-2 (#2)	-	liquid	100%	n.p.	-	12.4	Mild	Mild	Category 2A		Category II	R36	Swanson and Harbell (2000)					
1-3 (#3)	-	liquid	100%	n.p.	-	29.6	Moderate	Moderate	Category 2A		Category II	R36	Swanson and Harbell (2000)					
2-4 (#4)	-	liquid	100%	n.p.	-	7.3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Swanson and Harbell (2000)					
2-7 (#7)	-	liquid	100%	n.p.	-	21.4	Moderate	Moderate	Nonirritant		Category IV	Nonirritant	Swanson and Harbell (2000)					
2-8 (#8)	-	liquid	100%	n.p.	-	31.8	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Swanson and Harbell (2000)					
Acetone	67-64-1	liquid	100%	99	1	145.5	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)					
Acetone	67-64-1	liquid	100%	99	2	119.5	Very severe						Balls et al. (1995)					
Acetone	67-64-1	liquid	100%	99	3	120.4	Very severe						Balls et al. (1995)					
Acetone	67-64-1	liquid	100%	99	4	131.72	Very severe						Balls et al. (1995)					
Acetone	67-64-1	liquid	100%	99	5	98.4	Very severe						Balls et al. (1995)					
Acetone	67-64-1	liquid	100%	n.p.	-	-	Severe	Severe	Category 2A		Category II	R36	Casterton et al. (1996)					
Alkyl phosphoric acid ester/amine salt	-	liquid	100%	n.p.	-	91.3	Severe	Severe	Category 1	4	SCNM	R41	Bailey et al. (2004)					
All Purpose Cleaner (#5)	-	liquid	100%	n.p.	-	121.3	Severe	Severe					Swanson et al. (1995)					
All Purpose Cleaner (#7)	-	liquid	100%	n.p.	-	393.3	Severe	Severe					Swanson et al. (1995)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	1	156	Severe	Severe	Category 2A		Category III	R36	Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	2	138	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	3	232	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	4	156	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	5	132	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	6	191	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	7	190	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	8	166	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	9	123	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	10	101	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	11	200	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	12	90	Severe						Gautheron et al. (1994)					
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	1	5	Mild						Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	2	4	Mild											Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	3	10	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	4	3	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	5	5	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	6	28	Moderate	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	7	2	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	8	4	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	9	10	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	10	6	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	11	2	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	12	2	Mild	Gautheron et al. (1994)										
2-Aminophenol	95-55-6	solid	20%	n.p.	1	7	Mild	Mild	Nonirritant		Category IV	Nonirritant						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	2	5	Mild											Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	3	3	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	4	5	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	5	6	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	6	7	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	7	5	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	8	6	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	9	13	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	10	11	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	11	5	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	12	11	Mild						Gautheron et al. (1994)					
Ammonium nitrate	6484-52-2	solid	20%	>99.9	1	8.3	Mild											Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	2	6.4	Mild											Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	3	7.2	Mild	Balls et al. (1995)										

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Ammonium nitrate	6484-52-2	solid	20%	>99.9	4	21.82	Mild	Mild	Category 2B		Category III	R36	Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	5	5.2	Mild						Balls et al. (1995)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	1 (1)	4.9	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	1 (2)	5.9	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	2 (1)	3.9	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	2 (2)	3.6	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	3 (1)	5.2	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	3 (2)	6.7	Mild						Southee (1998)
Amway all fabric bleach	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway automatic dishwashing compound for soft water	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway automatic dishwashing compound, standard formula	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway concrete floor cleaner	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	SCNM	R41	Casterton et al. (1996)
Amway Dish Drops dishwashing liquid	-	n.p.	100%	n.p.	-	-	Moderate	Moderate					Casterton et al. (1996)
Amway dry chlorine bleach	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway fabric softener	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Amway Kool Wash delicate fabric detergent	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R36	Casterton et al. (1996)
Amway LOC all purpose cleaner	-	n.p.	100%	n.p.	-	-	Mild	Mild	SCNM		SCNM	Nonirritant	Casterton et al. (1996)
Amway prewash liquid	-	liquid	100%	n.p.	-	-	Mild	Mild	SCNM		Category I	Nonirritant	Casterton et al. (1996)
Amway Pursue disinfectant cleaner	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway Redu dye stain remover	-	n.p.	100%	n.p.	-	-	Mild	Mild	Category 2A		Category II	Nonirritant	Casterton et al. (1996)
Amway SA8 laundry liquid	-	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Amway SA8 limited phos laundry powder	-	solid	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Anthracene	120-12-7	solid	20%	n.p.	1	-2	Nonirritant	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	3	-3	Nonirritant						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	4	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	6	-1	Nonirritant						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	7	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	8	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	10	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	12	2	Mild						Gautheron et al. (1994)
Anti-Dandruff Shampoo (HZY)	-	n.p.	100%	n.p.	-	-	Moderate						Moderate
Anti-Dandruff Shampoo (HZY) 100%	-	n.p.	10%	n.p.	-	20.8	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Aromatic hydrocarbon #1	-	liquid	100%	n.p.	-	2.7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Aromatic hydrocarbon #2	-	liquid	100%	n.p.	-	4.6	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Aryl phosphonates	-	liquid	100%	n.p.	-	41.3	Moderate	Moderate	Category 2B		SCNM	SCNM	Bailey et al. (2004)
L-Aspartic acid	70-47-3	solid	20%	100	1	1.8	Mild	Mild	SCNM ¹¹		SCNM	SCNM	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	2	0.1	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	3	2.6	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	4	0.788	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	5	1.2	Mild						Balls et al. (1995)
Baby Shampoo No. 1 (HZZ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Baby Shampoo No. 1 (HZZ) 100%	-	n.p.	10%	n.p.	-	4.0	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Baby Shampoo No. 2 (HZF)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Baby Shampoo No. 2 (HZF) 100%	-	n.p.	10%	n.p.	-	8.3	Nonsevere	Nonsevere	Category 1	1	Category I	R41	Gettings et al. (1996)
Bathroom Cleaner (#6)	-	liquid	100%	n.p.	-	78.3	Severe	Severe	SCNM		Category III	Nonirritant	Swanson et al. (1995)
Benchmark-Group 1 (#12)	-	liquid	100%	n.p.	-	60.1	Severe	Severe	Category 2A		Category I	R36	Swanson and Harbell (2000)
Benchmark-Group 2 (#13)	-	liquid	100%	n.p.	-	60.1	Severe	Severe	Category 1	1	Category I	R41	Swanson and Harbell (2000)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (1)	195.2	Very severe	Very Severe	Category 1	4	SCNM	R41	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (2)	135.2	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (3)	137.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (4)	156.5	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (5)	138.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (6)	176.8	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (7)	183.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (8)	175.4	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (1)	154.4	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (2)	156.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (3)	150.8	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (4)	157.2	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (5)	157.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (6)	157.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (7)	160.2	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (1)	156.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (2)	163.4	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (3)	169.7	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (4)	162.8	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (5)	151.6	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (6)	163.1	Very severe	Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (7)	167.8	Very severe	Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (8)	156.9	Very severe	Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (9)	160.0	Very severe	Southee (1998)					
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	98	1	112.8	Very severe	Very Severe	Category 1	1	Category II	R41	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	98	2	90.5	Very severe						Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	98	3	99.4	Very severe						Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	98	4	62.49	Severe						Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	98	5	78.6	Severe						Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	n.p.	-	-	Severe	Severe	Category I	1	Category I	R41	Casterton et al. (1996)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	1	142.2	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	2	157.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	3	123.8	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	4	137.5	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	5	121.1	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	1	126.6	Very severe	Very Severe	Category 1	2	Category I	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	2	163.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	3	110.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	4	130.41	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	5	111.1	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	n.p.	-	-	Severe	Severe	Category 1	2	Category I	R41	Casterton et al. (1996)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	1	128	Severe	Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	2	124	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	3	163	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	4	106	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	5	128	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	6	129	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	7	142	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	8	129	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	9	166	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	10	no data	n.a. ¹³						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	11	142	Severe						Gautheron et al. (1994)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	12	116	Severe						Gautheron et al. (1994)					
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	1	173	Very severe	Very Severe	Category 1	2	SCNM	R41	Balls et al. (1995)					
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	2	288.7	Very severe						Balls et al. (1995)					
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	3	91.1	Very severe						Balls et al. (1995)					
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	4	149.86	Very severe						Balls et al. (1995)					
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	5	145.3	Very severe						Balls et al. (1995)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	1	4	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	3	0	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	4	1	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	5	1	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	6	3	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	8	-10	Nonirritant						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	9	4	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	10	-1	Nonirritant						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	11	1	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	1	0	Mild						Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	2	2	Mild											Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	3	-1	Nonirritant											Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	4	1	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	5	0	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	6	0	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	7	0	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	8	0	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	9	1	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	11	-2	Nonirritant	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	12	-2	Nonirritant	Gautheron et al. (1994)										
4-Bromophenetole	-	n.p.	100%	n.p.	-	-	Mild	Mild										Casterton et al. (1996)
Bubble Bath (HZK)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41						Casterton et al. (1996)
Bubble Bath (HZK) 100%	-	n.p.	100%	n.p.	-	17.5	Severe	Severe	Category 1	1	Category I	R41						Gettings et al. (1996)
n-Butanol	71-36-3	liquid	100%	n.p.	-	-	Severe	Severe					Casterton et al. (1996)					
2-Butoxyethanol	111-76-2	liquid	100%	n.p.	-	-	Severe	Severe					Casterton et al. (1996)					
Butyl acetate	123-86-4	liquid	100%	99	1	49.5	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)					
Butyl acetate	123-86-4	liquid	100%	99	2	37.5	Moderate						Balls et al. (1995)					
Butyl acetate	123-86-4	liquid	100%	99	3	43.9	Moderate						Balls et al. (1995)					
Butyl acetate	123-86-4	liquid	100%	99	4	23.86	Mild						Balls et al. (1995)					
Butyl acetate	123-86-4	liquid	100%	99	5	18.1	Mild						Balls et al. (1995)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	1 (1)	108.3	Very severe	Very Severe	Category 1	1	Category II	R41	Southee (1998)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	1 (2)	111.8	Very severe						Southee (1998)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	2 (1)	92.8	Very severe						Southee (1998)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	2 (2)	99.2	Very severe						Southee (1998)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	3 (1)	94.9	Very severe						Southee (1998)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	3 (2)	98.2	Very severe	Southee (1998)										
Butyrolactone	96-48-0	liquid	100%	n.p.	1	48	Moderate	Moderate	Category 2A		Category II	R36	Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	2	44	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	3	64	Severe						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	4	35	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	5	35	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	6	30	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	7	80	Severe						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	8	32	Moderate						Gautheron et al. (1994)					

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Butyrolactone	96-48-0	liquid	100%	n.p.	9	42	Moderate						Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	100%	n.p.	10	53	Moderate						Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	100%	n.p.	11	35	Moderate						Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	100%	n.p.	12	49	Moderate						Gautheron et al. (1994)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	1	90.6	Very severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	2	32.9	Moderate						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	3	31.5	Moderate						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	4	81.55	Very severe						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	5	67.1	Severe						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	1	27.8	Moderate	Moderate	Category 1	4	Category I	R41	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	2	27.2	Moderate						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	3	34.8	Moderate						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	4	102.918	Very severe						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	5	26.4	Moderate					Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1	97.6	Very severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2	98.1	Very severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3	57.5	Severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	4	64.33	Severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	5	73.9	Severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	100%	n.p.	-	-	Mild	Mild	Category 2A		Category II	R36	Casterton et al. (1996)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1 (1)	53.9	Moderate	Moderate	Category 2A		Category II	R36	Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1 (2)	47.7	Moderate						Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2 (1)	47.1	Moderate						Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2 (2)	47.2	Moderate						Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3 (1)	42.2	Moderate						Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3 (2)	41.8	Moderate	Southee (1998)					
Carboxylic acid amides	-	solid	100%	n.p.	-	27.5	Moderate	Moderate	Category 1	4	Category I	R41	Bailey et al. (2004)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	1	11	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	2	4.1	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	3	12.1	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	4	4.33	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	5	14.5	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0%	n.p.	-	-	Mild						Casterton et al. (1996)
Cetylpyridinium bromide (1%)	140-72-7	liquid	1%	n.p.	-	-	Moderate						Moderate
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	1	43.5	Moderate	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	2	89.6	Very severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	3	81	Very severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	4	71.22	Severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	5	76.7	Severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	1	72.2	Severe	Severe	Category 1	2	SCNM	R41	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	2	86.3	Very severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	3	63.6	Severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	4	68.72	Severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	5	65.4	Severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	n.p.	-	-	Severe	Severe	Category 1	2	SCNM	R41	Casterton et al. (1996)
Chlorhexidine	55-56-1	solid	20%	n.p. ¹²	1	147	Very severe	Very Severe	Category 1	4	SCNM	SCNM	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	2	122.9	Very severe						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	3	97.3	Very severe						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	4	101.78	Very severe						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	5	101.5	Very severe						Balls et al. (1995)
2-Chloro-2,4,4-trimethylpentane	-	liquid	100%	n.p.	-	4.1	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Clarified slurry oil	-	liquid	100%	n.p.	-	2.3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Cleaner/Degreaser (#13)	-	liquid	100%	n.p.	-	353.6	Severe	Severe					Swanson et al. (1995)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference	
Cleansing Gel (HZQ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)	
Cleansing Gel (HZQ) 100%	-	n.p.	10%	n.p.	-	2.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)	
Cutting fluid (conc.) #1	-	liquid	100%	n.p.	-	3.5	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)	
Cutting fluid (conc.) #2	-	liquid	100%	n.p.	-	4.9	Mild	Mild	Nonirritant		Category III	Nonirritant	Bailey et al. (2004)	
Cyclohexanol	108-93-0	liquid	100%	n.p.	97	1	85	Very severe					Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	100%	n.p.	97	2	49.9	Moderate					Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	100%	n.p.	97	3	70.1	Severe	Moderate	Category 1	2	Category I	R41	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	n.p.	97	4	52.24	Moderate					Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	100%	n.p.	97	5	43.2	Moderate					Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	100%	n.p.	-	-	Severe	Severe	Category 1	2	Category I	R41	Casterton et al. (1996)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	1	92	Severe						Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	2	108	Severe						Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	3	96	Severe						Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	4	81	Severe						Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	5	130	Severe						Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	6	93	Severe	Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	7	104	Severe						Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	8	90	Severe						Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	9	142	Severe						Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	11	118	Severe						Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	100%	n.p.	12	108	Severe						Gautheron et al. (1994)	
Degreaser (#16)	-	liquid	100%	n.p.	-	255.7	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	1	96	Severe						Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	2	72	Severe						Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	3	106	Severe						Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	4	73	Severe						Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	5	119	Severe						Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	6	103	Severe	Severe	Category 2A		Category II	R36	Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	7	88	Severe						Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	8	46	Moderate						Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	9	100	Severe						Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	10	60	Severe						Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	11	200	Severe						Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	12	59	Severe						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	1	53	Moderate						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	2	41	Moderate						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	3	105	Severe						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	4	39	Moderate						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	5	42	Moderate						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	6	34	Moderate						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	7	49	Moderate	Moderate	SCNM		SCNM	SCNM	Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	8	41	Moderate						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	9	92	Severe						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	11	36	Moderate						Gautheron et al. (1994)	
Diacetone alcohol	123-42-2	liquid	100%	n.p.	12	56	Severe						Gautheron et al. (1994)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	1	104	Severe						Gautheron et al. (1994)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	2	134	Severe						Gautheron et al. (1994)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	3	82	Severe						Gautheron et al. (1994)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	4	118	Severe						Gautheron et al. (1994)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	5	110	Severe						Gautheron et al. (1994)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	6	66	Severe	Severe	Category 1	2	Category I	R41	Gautheron et al. (1994)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	7	88	Severe						Gautheron et al. (1994)	

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	8	193	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	9	82	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	11	213	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	12	135	Severe						Gautheron et al. (1994)					
Dibenzyl phosphate	1623-08-1	solid	20%	99	1	304.1	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)					
Dibenzyl phosphate	1623-08-1	solid	20%	99	2	391.1	Very severe						Balls et al. (1995)					
Dibenzyl phosphate	1623-08-1	solid	20%	99	3	418	Very severe						Balls et al. (1995)					
Dibenzyl phosphate	1623-08-1	solid	20%	99	4	467.09	Very severe						Balls et al. (1995)					
Dibenzyl phosphate	1623-08-1	solid	20%	99	5	307.5	Very severe						Balls et al. (1995)					
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	1	9.9	Mild	Mild	Category 2A		Category II	SCNM	Balls et al. (1995)					
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	2	11.2	Mild						Balls et al. (1995)					
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	3	10.8	Mild						Balls et al. (1995)					
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	4	14.43	Mild						Balls et al. (1995)					
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	5	5.6	Mild						Balls et al. (1995)					
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	n.p.	-	-	Mild						Casterton et al. (1996)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	1	23	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	2	23	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	3	18	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	4	28	Moderate						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	5	16	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	6	31	Moderate						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	7	18	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	8	71	Severe						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	9	19	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	10	20	Mild						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	11	34	Moderate						Gautheron et al. (1994)					
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	12	14	Mild						Gautheron et al. (1994)					
2,4-Difluoronitrobenzene	446-35-5	liquid	100%	n.p.	-	-	Mild						Mild					Casterton et al. (1996)
1,3-Diisopropylbenzene	99-62-7	liquid	100%	n.p.	-	-	Mild						Mild					Casterton et al. (1996)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	1	0	Mild						Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	2	3	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	3	1	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	4	3	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	5	1	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	6	5	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	7	3	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	8	1	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	9	2	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	11	5	Mild	Gautheron et al. (1994)										
Dimethylbiguanide	657-24-9	solid	20%	n.p.	12	8	Mild	Gautheron et al. (1994)										
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	1	103.8	Very severe	Very Severe	SCNM		Category I	SCNM						Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	2	115	Very severe											Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	3	131.7	Very severe											Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	4	130.26	Very severe						Balls et al. (1995)					
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	5	78.8	Severe						Balls et al. (1995)					
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	n.p.	-	-	Severe	Severe	SCNM		Category I	SCNM	Casterton et al. (1996)					
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	1	18.2	Mild	Mild	Category I	1	Category I	R41	Balls et al. (1995)					
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	2	25.3	Moderate						Balls et al. (1995)					
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	3	20.5	Mild						Balls et al. (1995)					
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	4	31.533	Moderate						Balls et al. (1995)					
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	5	8.3	Mild						Balls et al. (1995)					
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	1	10	Mild						Gautheron et al. (1994)					

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	2	10	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	3	14	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	4	11	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	5	11	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	6	14	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	7	10	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	8	10	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	9	9	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	11	4	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	12	22	Mild						Gautheron et al. (1994)
Dodecane	112-40-3	liquid	100%	n.p.	-	-	Mild						Mild
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	1	-1	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	2	0	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	3	-8	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	4	2	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	5	2	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	6	2	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	8	-6	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	10	-1	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	11	3	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	12	1	Mild						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	1	74.4	Severe	Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	2	53.2	Moderate						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	3	63.3	Severe						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	4	98.01	Very severe						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	5	64.2	Severe						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	1	58	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	2	67	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	3	70	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	4	45	Moderate						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	5	60	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	6	64	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	7	58	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	8	51	Moderate	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	9	46	Moderate	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	11	104	Severe	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	12	45	Moderate	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	1 (1)	36.6	Moderate	Moderate	Category 2A		Category III	Nonirritant	Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	1 (2)	37.6	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (3)	29.6	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (4)	41.7	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (5)	31.5	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (6)	42.6	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (7)	55.4	Severe						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (1)	52.7	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (2)	54.5	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (3)	61.7	Severe						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (4)	60.2	Severe						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (5)	54.2	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (6)	73.4	Severe						Southee (1998)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Ethanol	64-17-5	liquid	100%	n.p.	2 (7)	64.0	Severe						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (8)	51.4	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (1)	47.0	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (2)	45.4	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (3)	44.4	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (4)	45.7	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (5)	54.6	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (6)	44.8	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (7)	42.2	Moderate						Southee (1998)
Ethanol (#14)	64-17-5	liquid	100%	n.p.	-	52.7	Moderate	Moderate	Category 2A		Category I	R36	Swanson and Harbell (2000)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	1	99	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	2	100	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	3	128	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	4	75	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	5	75	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	6	85	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	7	94	Severe	Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	8	93	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	9	84	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	10	75	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	11	101	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	12	86	Severe						Gautheron et al. (1994)
Ethyl acetate	141-78-6	liquid	100%	99	1	19.7	Mild						Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	2	28.4	Moderate						Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	3	47.1	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	4	44.31	Moderate						Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	5	20.6	Mild						Balls et al. (1995)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	1	26	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	2	38	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	3	31	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	4	33	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	5	21	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	6	29	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	7	28	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	8	38	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	9	26	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	11	38	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	12	42	Moderate						Gautheron et al. (1994)
2-Ethylhexanol	104-76-7	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 2A		Category II	R36	Casterton et al. (1996)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	1	62	Severe						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	2	28.2	Moderate						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	3	30.7	Moderate	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	4	58.71	Severe						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	5	19.6	Mild						Balls et al. (1995)
Ethylhexyl acid phosphate ester	-	liquid	100%	n.p.	-	130.5	Severe	Severe	Category 1	4	SCNM	R41	Bailey et al. (2004)
5-Ethylidene-2-norbornene	16219-75-3	liquid	100%	n.p.	-	8.8	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	1	27.5	Moderate						Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	2	14.1	Mild						Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	3	5.5	Mild	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	4	5.543	Mild						Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	5	19.6	Mild						Balls et al. (1995)
3-Ethyltoluene	620-14-4	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	1	27.4	Moderate						Balls et al. (1995)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	2	33.7	Moderate	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	3	10.5	Mild						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	4	8.633	Mild						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	5	9	Mild						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	n.p.	-	-	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Eye Make-Up Remover (HZH)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Eye Make-Up Remover (HZH) 100%	-	n.p.	10%	n.p.	-	0.2	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Facial Cleansing Foam (HZR) 25%	-	n.p.	10%	n.p.	-	4.1	Nonsevere	Nonsevere	Nonsevere	SCNM	Category I	SCNM	Gettings et al. (1996)
Facial Cleanser (HZZ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Facial Cleanser (HZZ) 100%	-	n.p.	10%	n.p.	-	1.8	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Floor Cleaner (#10)	-	liquid	100%	n.p.	-	70.3	Severe	Severe					Swanson et al. (1995)
Floor Cleaner (#2)	-	liquid	100%	n.p.	-	-0.3	Nonirritant	Nonirritant					Swanson et al. (1995)
Floor Stripper (#14)	-	liquid	100%	n.p.	-	157.3	Severe	Severe					Swanson et al. (1995)
Floor Stripper (#17)	-	liquid	100%	n.p.	-	216.2	Severe	Severe	Category 1	NC	Category I	R41	Swanson et al. (1995)
Floor Stripper (#18)	-	liquid	100%	n.p.	-	444.3	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Foam Bath (HZL)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Foam Bath (HZL) 100%	-	n.p.	10%	n.p.	-	18.6	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Fomesafen	72128-02-0	solid	20%	97.5	1	45.5	Moderate	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	2	151.9	Very severe						Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	3	64.9	Severe						Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	4	23.023	Mild						Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	5	18.2	Mild						Balls et al. (1995)
Furan	110-00-9	liquid	100%	n.p.	1	73	Severe	Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	2	63	Severe						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	3	61	Severe						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	4	65	Severe						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	5	33	Moderate						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	6	34	Moderate						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	7	87	Severe						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	8	48	Moderate						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	9	50	Moderate						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	10	39	Moderate						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	11	68	Severe						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	12	51	Moderate						Gautheron et al. (1994)
Gel Cleanser (HZE)	-	n.p.	100%	n.p.	-	-	Mild	Mild	SCNM		Category I	SCNM	Casterton et al. (1996)
Gel Cleanser (HZE) 100%	-	n.p.	10%	n.p.	-	3.1	Nonsevere	Nonsevere	SCNM		Category I	SCNM	Gettings et al. (1996)
General Cleaner (#11)	-	liquid	100%	n.p.	-	83.3	Severe	Severe					Swanson et al. (1995)
General Cleaner (#12)	-	liquid	100%	n.p.	-	113.5	Severe	Severe					Swanson et al. (1995)
Glass Cleaner (#19)	-	liquid	100%	n.p.	-	135.8	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Gluconolactone	90-80-2	solid	20%	n.p.	1	63	Severe	Severe	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	2	81	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	3	90	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	4	62	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	5	108	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	6	66	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	7	90	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	8	57	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	9	88	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	11	75	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	12	63	Severe						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	1	2	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	3	1	Mild						Gautheron et al. (1994)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	4	1	Mild	Mild	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	6	-4	Nonirritant						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	8	4	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	9	0	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	10	2	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	11	0	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	12	-1	Nonirritant						Gautheron et al. (1994)					
Glycerol	56-81-5	liquid	100%	>99.5	1	-2	Mild						Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	2	-0.2	Mild											Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	3	0.3	Mild											Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	4	3.08	Mild	Balls et al. (1995)										
Glycerol	56-81-5	liquid	100%	>99.5	5	0.1	Mild	Balls et al. (1995)										
Glycerol	56-81-5	liquid	100%	n.p.	-	-	Mild	Casterton et al. (1996)										
Glycerol	56-81-5	liquid	100%	>99.5	1 (1)	0.6	Mild	Nonirritant	Nonirritant		Category IV	Nonirritant	Southee (1998)					
Glycerol	56-81-5	liquid	100%	>99.5	1 (2)	0.3	Mild						Southee (1998)					
Glycerol	56-81-5	liquid	100%	>99.5	2 (1)	0.8	Nonirritant						Southee (1998)					
Glycerol	56-81-5	liquid	100%	>99.5	2 (2)	0.8	Nonirritant						Southee (1998)					
Glycerol	56-81-5	liquid	100%	>99.5	3 (1)	1.0	Nonirritant						Southee (1998)					
Glycerol	56-81-5	liquid	100%	>99.5	3 (2)	0.8	Nonirritant						Southee (1998)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	1	18	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	2	24	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	3	25	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	4	14	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	5	13	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	6	6	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	7	15	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	8	18	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	9	18	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	10	4	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	11	23	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	12	21	Mild						Gautheron et al. (1994)					
Hand Soap (HZU) 25%	-	n.p.	10%	n.p.	-	5.5	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Heavy Duty Cleaner (#15)	-	liquid	100%	n.p.	-	357.1	Severe	Severe	Category 1	NC	Category I	R41	Swanson et al. (1995)					
Heavy Duty Cleaner/Degreaser (#9)	-	liquid	100%	n.p.	-	354.7	Severe	Severe	Category 1				Swanson et al. (1995)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1	93	Severe	Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2	40	Moderate						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3	53	Moderate						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	4	33	Moderate						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	5	91	Severe						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	6	42	Moderate						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	7	82	Severe						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	8	76	Severe						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	9	70	Severe						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	11	48	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	12	102	Severe						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1 (1)	23.1	Mild	Moderate	Category 1	4	Category I	R41	Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1 (2)	17.2	Mild						Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2 (1)	34.6	Moderate						Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2 (2)	39.1	Moderate						Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3 (1)	31.7	Moderate						Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3 (2)	29.9	Moderate						Southee (1998)
1,5-Hexadiene	592-42-7	liquid	100%	n.p.	-	-	Mild						Mild
Hexane	110-54-3	liquid	100%	n.p.	1	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	2	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	3	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	4	0	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	5	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	6	1	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	7	3	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	8	1	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	9	1	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	10	-1	Nonirritant						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	12	6	Mild						Gautheron et al. (1994)
n-Hexanol	111-27-3	liquid	100%	98	1	71.5	Severe						Severe/Very Severe
n-Hexanol	111-27-3	liquid	100%	98	2	83.6	Very severe	Balls et al. (1995)					
n-Hexanol	111-27-3	liquid	100%	98	3	63.2	Severe	Balls et al. (1995)					
n-Hexanol	111-27-3	liquid	100%	98	4	48.19	Moderate	Balls et al. (1995)					
n-Hexanol	111-27-3	liquid	100%	98	5	42.9	Moderate	Balls et al. (1995)					
Imidazole	288-32-4	solid	20%	99	1	116.8	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	2	133.9	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	3	103.4	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	4	118.7	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	5	90.8	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	n.p.	1	75	Severe	Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	2	73	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	3	140	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	4	81	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	5	96	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	6	62	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	7	82	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	8	122	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	9	64	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	10	81	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	11	114	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	12	65	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	1 (1)	142.0	Very severe						
Imidazole	288-32-4	solid	20%	n.p.	1 (2)	137.6	Very severe						Southee (1998)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Imidazole	288-32-4	solid	20%	n.p.	1 (3)	112.2	Very severe	Very Severe	Category 1	4	Category I	R41	Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	1 (4)	131.1	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	1 (5)	145.6	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	1 (6)	162.6	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	1 (7)	125.5	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (1)	138.1	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (2)	140.1	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (3)	134.9	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (4)	157.2	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (5)	137.6	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (6)	152.9	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (7)	148.7	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (1)	139.6	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (2)	140.1	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (3)	124.0	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (4)	128.7	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (5)	123.4	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (6)	121.2	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (7)	131.3	Very severe						Southee (1998)
Iminodibenzyl	494-19-9	solid	20%	n.p.	1	0	Mild						Mild
Iminodibenzyl	494-19-9	solid	20%	n.p.	2	1	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	3	6	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	4	0	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	5	4	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	6	0	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	7	1	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	8	12	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	9	0	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	10	no data	n.a.	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	11	6	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	12	-4	Nonirritant	Gautheron et al. (1994)					
Isobutanol	78-83-1	liquid	100%	99.9	1	54.4	Moderate	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	2	74	Severe						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	3	67.7	Severe						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	4	41.78	Moderate						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	5	42.2	Moderate	Severe	Category 2A		Category II	R36	Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	n.p.	-	-	Severe						Casterton et al. (1996)
Isopropanol	67-63-0	liquid	100%	99.9	1	39.7	Moderate	Severe	Category 2A		Category III	SCNM	Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	2	59.5	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	3	72.3	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	4	78.5	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	5	39.3	Moderate						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	n.p.	-	-	Moderate						Casterton et al. (1996)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	1	53	Moderate	Moderate	Category 2B		Category III	Nonirritant	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	2	50	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	3	48	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	4	28	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	5	45	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	6	35	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	7	48	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	8	43	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	9	63	Severe						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	11	89	Severe	Severe	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	12	48	Moderate						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	1	81	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	2	82	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	3	103	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	4	76	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	5	92	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	6	68	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	7	90	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	8	62	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	9	102	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	11	76	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	12	55	Moderate						Gautheron et al. (1994)					
Liquid Soap No. 2 (HZW) 25%	-	n.p.	10%	n.p.	-	5.6	Nonsevere						Nonsevere	Category 2B		Category III	Nonirritant	Gettings et al. (1996)
Liquid Soap No. 1 (HZB) 25%	-	n.p.	10%	n.p.	-	2.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	1	3	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	2	6	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	3	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	4	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	6	1	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	7	7	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	8	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	11	0	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)					
Maneb	12427-38-2	solid	20%	90	1	67	Severe						Nonsevere	SCNM		Category III	SCNM	Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	2	16.9	Mild											Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	3	21	Mild											Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	4	63.76	Severe	Balls et al. (1995)										
Maneb	12427-38-2	solid	20%	90	5	33.8	Moderate	Balls et al. (1995)										
Meat Room Degreaser (#3)	-	liquid	100%	n.p.	-	140.3	Severe	Severe				R41	Swanson et al. (1995)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	1	0	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	2	-1	Nonirritant						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	3	-1	Nonirritant						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	4	1	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	6	1	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	7	0	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	8	-8	Nonirritant						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	9	0	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	10	0	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	11	-4	Nonirritant						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	12	-3	Nonirritant						Gautheron et al. (1994)					
Metal Cleaner (#20)	-	liquid	100%	n.p.	-	391.9	Severe	Severe	Category 1	4	Category 1	R41	Swanson et al. (1995)					
Methanol	67-56-1	liquid	100%	n.p.	1	88	Severe	Severe	Nonirritant		Category II	Nonirritant	Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	2	88	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	3	54	Moderate						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	4	71	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	5	81	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	6	108	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	7	37	Moderate						Gautheron et al. (1994)					

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Methanol	67-56-1	liquid	100%	n.p.	8	19	Mild						Gautheron et al. (1994)
Methanol	67-56-1	liquid	100%	n.p.	9	99	Severe						Gautheron et al. (1994)
Methanol	67-56-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Methanol	67-56-1	liquid	100%	n.p.	11	179	Severe						Gautheron et al. (1994)
Methanol	67-56-1	liquid	100%	n.p.	12	102	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	1	61	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	2	69	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	3	66	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	4	47	Moderate						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	5	48	Moderate						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	6	62	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	7	65	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	8	62	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	9	57	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	11	74	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	12	88	Severe						Gautheron et al. (1994)
Methyl acetate	79-20-9	liquid	100%	98	1	71.2	Severe						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	2	46.5	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	3	51.6	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	4	53.9	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	5	51.1	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	n.p.	-	-	Moderate						Casterton et al. (1996)
Methyl cyanoacetate	105-34-0	liquid	100%	99	1	16.3	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	2	5.9	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	3	10.1	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	4	17.53	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	5	11	Mild						Balls et al. (1995)
Methyl cyclopentadiene dimer	-	liquid	100%	n.p.	-	0.7	Mild						Bailey et al. (2004)
Methylcyclopentane	96-37-7	liquid	100%	>99	1	3.8	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	2	4.6	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	3	1.4	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	4	1.71	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	5	2.7	Mild						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	1	93	Very severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	2	67.4	Severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	3	52.2	Moderate						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	4	78.71	Severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	5	60.8	Severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	n.p.	-	-	Moderate						Casterton et al. (1996)
Methyl ethyl ketone	78-93-3	liquid	100%	99	1 (1)	73.3	Severe						Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	100%	99	1 (2)	67.8	Severe						Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	100%	99	2 (1)	108.7	Very severe						Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	100%	99	2 (2)	101.7	Very severe						Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	100%	99	3 (1)	70.2	Severe						Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	100%	99	3 (2)	73.5	Severe						Southee (1998)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	1	8.8	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	2	20.1	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	3	10.3	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	4	13.25	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	5	10.3	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	n.p.	-	-	Moderate						Casterton et al. (1996)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	1	22	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	2	25	Mild						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	3	27	Moderate	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	4	19	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	5	21	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	6	23	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	7	16	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	8	16	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	9	19	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	11	20	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	12	11	Mild						Gautheron et al. (1994)
1-Methylpropyl benzene	135-98-8	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Mild Shampoo (HZJ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Mild Shampoo (HZJ) 25%	-	n.p.	10%	n.p.	-	0.1	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
MYRJ-45	-	surfactant	10%	n.p.	1	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	2	1	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	3	0	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	4	1	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	5	0	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	6	0	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	7	1	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	8	-4	Nonirritant						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	9	1	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	11	-3	Nonirritant						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	12	-1	Nonirritant						Gautheron et al. (1994)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	1	120.8	Very severe						Very Severe
1-Naphthalene acetic acid	86-87-3	solid	20%	96	2	66.3	Severe	Balls et al. (1995)					
1-Naphthalene acetic acid	86-87-3	solid	20%	96	3	42	Moderate	Balls et al. (1995)					
1-Naphthalene acetic acid	86-87-3	solid	20%	96	4	88.73	Very severe	Balls et al. (1995)					
1-Naphthalene acetic acid	86-87-3	solid	20%	96	5	72.5	Severe	Balls et al. (1995)					
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	1	136	Very severe	Balls et al. (1995)					
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	2	144.9	Very severe	Very Severe	Category 1	1	Category I	R41	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	3	161	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	4	161.2	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	5	143	Very severe						Balls et al. (1995)
1-Nitropropane	108-03-2	liquid	100%	n.p.	1	11	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	2	8	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	3	9	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	4	4	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	5	6	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	6	7	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	7	6	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	8	6	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	9	17	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	10	4	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	11	6	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	12	7	Mild						Gautheron et al. (1994)
n-Octanol	111-87-5	liquid	100%	>99	1	43.4	Moderate	Moderate	Category 2B		Category II	R36	Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	2	78.9	Severe						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	3	39.8	Moderate						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	4	14.54	Mild						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	5	28	Moderate						Balls et al. (1995)
Octanol	111-87-5	liquid	100%	n.p.	1	65	Severe						Gautheron et al. (1994)
Octanol	111-87-5	liquid	100%	n.p.	2	33	Moderate	Gautheron et al. (1994)					

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Octanol	111-87-5	liquid	100%	n.p.	3	42	Moderate	Moderate	Category 2B		Category III	R36	Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	4	49	Moderate						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	5	66	Severe						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	6	48	Moderate						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	7	37	Moderate						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	8	25	Mild						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	9	61	Severe						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	11	31	Moderate						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	12	64	Severe						Gautheron et al. (1994)					
Parafluoraniiline	371-40-4	liquid	100%	99	1	29.5	Moderate						Moderate	SCNM		SCNM	Balls et al. (1995)	
Parafluoraniiline	371-40-4	liquid	100%	99	2	26.4	Moderate	Balls et al. (1995)										
Parafluoraniiline	371-40-4	liquid	100%	99	3	40.8	Moderate	Balls et al. (1995)										
Parafluoraniiline	371-40-4	liquid	100%	99	4	31.82	Moderate	Balls et al. (1995)										
Parafluoraniiline	371-40-4	liquid	100%	99	5	23.5	Moderate	Balls et al. (1995)										
Parafluoraniiline	371-40-4	liquid	100%	n.p.	-	-	Moderate	Casterton et al. (1996)										
Parafluoraniiline	371-40-4	liquid	100%	99	1 (1)	31	Moderate	Southee (1998)										
Parafluoraniiline	371-40-4	liquid	100%	99	1 (2)	35	Moderate	Southee (1998)										
Parafluoraniiline	371-40-4	liquid	100%	99	2 (1)	38.3	Moderate	Southee (1998)										
Parafluoraniiline	371-40-4	liquid	100%	99	2 (2)	37.5	Moderate	Southee (1998)										
Parafluoraniiline	371-40-4	liquid	100%	99	3 (1)	22.1	Mild	Southee (1998)										
Parafluoraniiline	371-40-4	liquid	100%	99	3 (2)	28.9	Moderate	Southee (1998)										
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	1	61	Severe	Severe	Nonirritant		Category III	Nonirritant					Gautheron et al. (1994)	
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	2	79	Severe										Gautheron et al. (1994)	
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	3	75	Severe										Gautheron et al. (1994)	
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	4	34	Moderate										Gautheron et al. (1994)	
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	5	70	Severe						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	6	46	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	7	54	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	8	44	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	9	50	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	10	67	Severe						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	11	62	Severe						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	12	76	Severe						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	1	8	Mild						Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	100%	n.p.	2	13	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	3	11	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	4	1	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	5	2	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	6	5	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	7	7	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	8	0	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	9	2	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	10	3	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	11	5	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	12	9	Mild	Gautheron et al. (1994)										
Petroleum wax	-	solid	100%	n.p.	-	0.3	Mild	Mild	Nonirritant		Category IV	Nonirritant						Bailey et al. (2004)
Phenylbutazone	50-33-9	solid	20%	n.p.	1	0	Mild	Mild	Nonirritant		Category IV	Nonirritant						Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	3	1	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	4	0	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	6	1	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	7	0	Mild						Gautheron et al. (1994)					

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Phenylbutazone	50-33-9	solid	20%	n.p.	8	-6	Nonirritant						Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	10	1	Mild						Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	11	-3	Nonirritant						Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	12	2	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	1	7	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	2	12	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	3	15	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	4	9	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	5	28	Moderate						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	6	6	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	7	6	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	8	16	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	9	13	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	10	15	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	11	13	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	12	15	Mild						Gautheron et al. (1994)
Polishing Scrub (H2T)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Polishing Scrub (H2T) 100%	-	n.p.	10%	n.p.	-	3.7	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Polyalkenylsuccinate ester/amine salt	-	liquid	100%	n.p.	-	2.3	Mild	Mild	SCNM		Category III	SCNM	Bailey et al. (2004)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	1	0.6	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	2	2.5	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	3	-1.3	Nonirritant						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	4	1.08	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	5	2.8	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Polyethylene glycol 600	-	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Pot and Pan Cleaner (#8)	-	liquid	100%	n.p.	-	-0.6	Nonirritant	Nonirritant					Swanson et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	1	16.2	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	2	22.9	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	3	12	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	4	17.38	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	5	6.5	Mild						Balls et al. (1995)
Process oil	-	liquid	100%	n.p.	-	2.7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Promethazine hydrochloride	58-33-3	solid	20%	98	1	120.3	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	2	84.2	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	3	125.7	Very severe	Very Severe	Category 1	3	Category I	R41	Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	4	123.09	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	5	153.8	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	1	117	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	2	156	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	3	109	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	4	111	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	5	164	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	6	174	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	7	103	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	8	50	Moderate						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	9	139	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	11	94	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	12	19	Mild						Gautheron et al. (1994)
Propylene glycol	57-55-6	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	1	7	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	2	7	Mild						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	3	14	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	4	4	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	5	6	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	6	9	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	7	6	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	8	11	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	9	6	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	11	12	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	12	5	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	1 (1)	11.2	Mild	Mild	Nonirritant		Category III	Nonirritant	Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	1 (2)	7.4	Mild						Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	2 (1)	5.2	Mild						Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	2 (2)	3.6	Mild						Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	3 (1)	7.7	Mild						Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	3 (2)	6.2	Mild	Southee (1998)					
Pyridine	110-86-1	liquid	100%	>99.9	1	140.7	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	2	145.4	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	3	132.4	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	4	199.02	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	5	122.7	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	n.p.	1	102	Severe	Severe	Category 1	4	Category II	R41	Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	2	123	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	3	186	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	4	79	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	5	102	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	6	77	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	7	124	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	8	132	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	9	105	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	11	96	Severe	Gautheron et al. (1994)					
Pyridine	110-86-1	liquid	100%	n.p.	12	115	Severe	Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	1	0.3	Mild	Mild	Category 1	1	Category I	R41	Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	2	0.4	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	3	2.1	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	4	1.85	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	5	3.1	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	1	17	Mild	Moderate	Category 1	1	Category I	R41	Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	2	29	Moderate						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	3	8	Mild						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	4	46	Moderate						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	5	52	Moderate						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	6	24	Mild						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	7	15	Moderate						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	8	18	Moderate						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	9	58	Severe						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	11	3	Mild	Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	12	72	Severe	Gautheron et al. (1994)					
Shampoo No. 1 (HZC) 25%	-	n.p.	10%	n.p.	-	30.0	Severe	Severe	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	10%	n.p.	-	14.0	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Shampoo No. 3 (HZM) 25%	-	n.p.	10%	n.p.	-	4.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Shampoo No. 4 (HZV) 25%	-	n.p.	10%	n.p.	-	8.4	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Shampoo No. 5 (HZD) 25%	-	n.p.	10%	n.p.	-	2.7	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Shampoo No. 6 (HZN) 25%	-	n.p.	10%	n.p.	-	4.5	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Shampoo No. 7 (HZA)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)					
Shampoo No. 7 (HZA) 100%	-	n.p.	10%	n.p.	-	6.6	Nonsevere	Nonsevere	Category 1	1	Category I	R41	Gettings et al. (1996)					
Shampoo No. 8 (HZG) 25%	-	n.p.	10%	n.p.	-	2.7	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Shower Gel (HZS)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)					
Shower Gel (HZS) 100%	-	n.p.	10%	n.p.	-	35.9	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)					
Skin Cleanser (HZI)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)					
Skin Cleanser (HZI) 100%	-	n.p.	10%	n.p.	-	15.8	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	1	167.4	Very severe	Very Severe	Category 2B		Category III	R36	Balls et al. (1995)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	2	133.2	Very severe						Balls et al. (1995)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	3	146.5	Very severe						Balls et al. (1995)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	4	171.08	Very severe						Balls et al. (1995)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	5	132.3	Very severe						Balls et al. (1995)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	n.p.	-	-	Severe	Severe	Category 2B		Category III	R36	Casterton et al. (1996)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	1	285.2	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	2	224.1	Very severe						Balls et al. (1995)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	3	254.7	Very severe						Balls et al. (1995)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	4	348.27	Very severe						Balls et al. (1995)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	5	247.2	Very severe						Balls et al. (1995)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	1 (1)	245.0	Very severe	Very Severe	Category 1	4	Category I	R41	Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	1 (2)	227.1	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	2 (1)	241.3	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	2 (2)	235.5	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	3 (1)	193.1	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	3 (2)	214.9	Very severe						Southee (1998)					
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	1	47.3	Moderate						Severe	Category 1	NC	Category I	R36	Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	2	93	Very severe											Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	3	63.2	Severe											Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	4	59.61	Severe											Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	5	53.3	Moderate	Balls et al. (1995)										
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	n.p.	-	-	Moderate	Moderate	Category 1	NC	Category I	R36	Casterton et al. (1996)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	1 (1)	5.4	Mild	Mild	Category 1	NC	Category I	SCNM	Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	1 (2)	5.2	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	2 (1)	15.9	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	2 (2)	17.3	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	3 (1)	8.7	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	3 (2)	5.6	Mild						Southee (1998)					
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	1	31.7	Moderate						Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	2	31.7	Moderate											Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	3	27.3	Moderate	Balls et al. (1995)										
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	4	26.22	Moderate	Balls et al. (1995)										
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	5	12.3	Mild	Balls et al. (1995)										
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)					
Sodium lauryl sulfate (30 %)	151-21-3	liquid	30%	n.p.	-	-	Moderate	Moderate					Casterton et al. (1996)					
Sodium oxalate	62-76-0	solid	20%	>99	1	2.1	Mild	Mild	Category 1	4	Category I	R41	Balls et al. (1995)					
Sodium oxalate	62-76-0	solid	20%	>99	2	7.6	Mild						Balls et al. (1995)					
Sodium oxalate	62-76-0	solid	20%	>99	3	5.8	Mild						Balls et al. (1995)					
Sodium oxalate	62-76-0	solid	20%	>99	4	49.59	Moderate						Balls et al. (1995)					
Sodium oxalate	62-76-0	solid	20%	>99	5	4.9	Mild						Balls et al. (1995)					
Sodium oxalate	62-76-0	solid	20%	n.p.	1	2	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	2	2	Mild						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Sodium oxalate	62-76-0	solid	20%	n.p.	3	9	Mild	Mild	Category 1	4	Category I	R41	Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	4	5	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	5	3	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	6	2	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	7	4	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	8	3	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	9	3	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	10	9	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	11	11	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	12	4	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	99	1 (1)	10.3	Mild						Nonirritant	Category 1	4	Category I	R41	Southee (1998)
Sodium oxalate	62-76-0	solid	20%	99	1 (2)	4.4	Mild	Southee (1998)										
Sodium oxalate	62-76-0	solid	20%	99	2 (1)	-0.3	Nonirritant	Southee (1998)										
Sodium oxalate	62-76-0	solid	20%	99	2 (2)	-0.1	Nonirritant	Southee (1998)										
Sodium oxalate	62-76-0	solid	20%	99	3 (1)	2.7	Nonirritant	Southee (1998)										
Sodium oxalate	62-76-0	solid	20%	99	3 (2)	4.5	Mild	Southee (1998)										
Sodium perborate	10486-00-7	solid	20%	98.6	1	143.6	Very severe	Very Severe	Category 1	4	Category I	R41						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	2	118.4	Very severe											Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	3	96.2	Very severe											Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	4	64.531	Severe											Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	5	62.9	Severe											Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	1	23.6	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	2	7.9	Mild						Balls et al. (1995)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	3	14.2	Mild						Balls et al. (1995)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	4	20.65	Mild						Balls et al. (1995)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	5	8.9	Mild						Balls et al. (1995)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	1	5	Mild	Mild	Nonirritant		Category II	Nonirritant	Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	3	2	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	4	6	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	6	4	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	7	2	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	8	19	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	9	3	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	11	18	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)					
Thiadiazole alkyl derivative	-	liquid	100%	n.p.	-	10.9	Moderate						Moderate	SCNM		Category III	SCNM	Bailey et al. (2004)
Thiourea	62-56-6	solid	20%	>99	1	149.4	Very severe	Very Severe	Animal died		Animal died	Animal died	Balls et al. (1995)					
Thiourea	62-56-6	solid	20%	>99	2	139.2	Very severe						Balls et al. (1995)					
Thiourea	62-56-6	solid	20%	>99	3	135.6	Very severe						Balls et al. (1995)					
Thiourea	62-56-6	solid	20%	>99	4	137.44	Very severe						Balls et al. (1995)					
Thiourea	62-56-6	solid	20%	>99	5	99.1	Very severe						Balls et al. (1995)					
Thiourea	62-56-6	solid	20%	n.p.	1	146	Severe	Severe	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	2	175	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	3	169	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	4	152	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	5	140	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	6	120	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	7	129	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	8	173	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	9	151	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Thiourea	62-56-6	solid	20%	n.p.	11	203	Severe						Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	12	104	Severe						Gautheron et al. (1994)
Toilet Bowl Cleaner (#1)	-	liquid	100%	n.p.	-	13.5	Mild	Mild	Nonirritant		Category IV	Nonirritant	Swanson et al. (1995)
Toilet Bowl Cleaner (#4)	-	liquid	100%	n.p.	-	15	Mild	Mild	Nonirritant		SCNM	Nonirritant	Swanson et al. (1995)
Toluene	108-88-3	liquid	100%	99	1	43.3	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	2	33.2	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	3	37.2	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	4	38.41	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	5	26.1	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	n.p.	-	-	Severe	Severe	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	1	81.9	Very severe	Severe/Very Severe	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	2	49.8	Moderate						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	3	75.3	Severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	4	92.97	Very severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	5	79.3	Severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	1	272	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	2	225	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	3	296.9	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	4	323.08	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	5	203.7	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	1	47	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	2	42	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	3	78	Severe						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	4	28	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	5	42	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	6	47	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	7	48	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	8	24	Mild						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	9	91	Severe						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	11	28	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	12	47	Moderate						Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	100%	n.p.	1	2	Mild						Mild
Triethanolamine	102-71-6	liquid	100%	n.p.	2	4	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	3	0	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	4	0	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	5	-1	Nonirritant	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	6	1	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	7	1	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	8	3	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	9	3	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	11	5	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	12	6	Mild	Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	1	25	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	2	14	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	3	26	Moderate						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	4	11	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	5	27	Moderate						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	6	7	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	7	9	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	8	15	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	9	21	Mild						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	10	10	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	11	7	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	12	21	Mild						Gautheron et al. (1994)
Triton X-100 (1%)	9002-93-1	liquid	1%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	1	85.7	Very severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	2	76	Severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	3	86.1	Very severe	Severe/Very Severe	Category 1	NC	Category II	R41	Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	4	57.58	Severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	5	46.2	Moderate						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	NC	Category II	R41	Casterton et al. (1996)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	1	74.3	Severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	2	106.6	Very severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	3	80.2	Very severe	Very Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	4	76.79	Very severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	5	53.6	Moderate						Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	5%	n.p.	-	-	Moderate	Moderate	Category 2A		Category III	Nonirritant	Casterton et al. (1996)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	1 (1)	3.7	Mild						Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	1 (2)	1.8	Mild						Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	2 (1)	5.8	Mild	Mild	Category 2B		Category III	R36	Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	2 (2)	3.4	Mild						Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	3 (1)	3.0	Nonirritant						Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	3 (2)	1.9	Nonirritant						Southee (1998)
Triton X-155	9010-44-0	surfactant	10%	n.p.	1	-1	Nonirritant						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	2	1	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	3	-1	Nonirritant						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	4	0	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	5	2	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	6	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	7	0	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	8	2	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	9	3	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	12	0	Mild						Gautheron et al. (1994)
Tween 20	9005-64-5	liquid	n.p.	98	1	-0.6	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	2	-1.1	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	3	-1.6	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	4	2.711	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	5	0.4	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	100%	98	1 (1)	0.3	Mild						Southee (1998)
Tween 20	9005-64-5	liquid	100%	98	1 (2)	0.0	Mild						Southee (1998)
Tween 20	9005-64-5	liquid	100%	98	2 (1)	0.4	Mild	Nonirritant	Nonirritant		Category III	Nonirritant	Southee (1998)
Tween 20	9005-64-5	liquid	100%	98	2 (2)	0.4	Nonirritant						Southee (1998)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Tween 20	9005-64-5	liquid	100%	98	3 (1)	0.3	Nonirritant						Southee (1998)
Tween 20	9005-64-5	liquid	100%	98	3 (2)	0.0	Nonirritant						Southee (1998)
Tween 20	9005-64-5	liquid	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Xylene	1330-20-7	liquid	100%	n.p.	-	-	Moderate	Moderate	Nonirritant		Category II	Nonirritant	Casterton et al. (1996)

¹CASRN=Chemical Abstract Services Registry Number

²*In Vitro* Classification represents the BCOP ocular irritancy classification assigned for each chemical in the study for each test for a specific substance

³Consensus classification represents the overall BCOP ocular irritancy classification assigned for each chemical in the study based on the majority of ocular irritancy classification calls

⁴GHS=Globally Harmonized System (UN [2003])

⁵Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye

⁶NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are both severe and persistent; and 4: corneal opacity score equal to 4 at any time; NC: not classified because none of the above criteria were met

⁷EPA=U.S. Environmental Protection Agency (EPA [1996]).

⁸Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 1-7 days; Category IV: minimal effects clearing in less than 24 hr

⁹EU=European Union (EU [2001]).

¹⁰Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

¹¹SCNM=Study Criteria Not Met

¹²n.p.=Not provided

¹³n.a.=Not applicable