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Cosmetics Europe compilation of historical serious eye damage/eye irritation *in vivo* data analysed by drivers of classification to support the selection of chemicals for development and evaluation of alternative methods/strategies: the Draize eye test Reference Database (DRD)

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Supplementary Material 1 (Archives of Toxicology)

Draize eye test Reference Database (DRD)

Cosmetics Europe
Draize eye test Reference Database (DRD)
Barroso *et al.* , 2016

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
1	2-Hydroxy iso-butyric acid ethyl ester	80-55-7	Alcohol| Carboxylic acid ester	L	Y	ZEBET	Sigma-Aldrich	98%	1 of 1	Cat 1	**CO mean ≥ 3**	3/3	Unknown				Study terminated on D3	
2	3-Diethylaminopropionitrile	5351-04-2	Aliphatic Amine, tertiary| Nitrile	L	Y	ECETOC	Chem Service, Inc.	98%	1 of 1	Cat 1	**CO mean ≥ 3**	2/3	Unknown		CO = 4	3/3	CO = 4 between D1 and D3 in 1/3 that reverts to CO ≤ 2 on D7 with study terminated on D7 with CC = 4; CO = 4 between D1 and D2 in 1/3 fully reversed by D7; CO = 4 on D1 in 1/3 fully reversed by D7	
3	Benzensulphonylchloride	98-09-9	Aryl| Sulfonyl halide	L	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	Cat 1	**CO mean ≥ 3**; IR mean > 1.5	4/6; 4/6	CO pers D21; Conj pers D21	at least 5/6; at least 4/6	CO = 4	5/6	CO = 4 between D3 and D7 and on D14 with CO = 2 on D21 and D24, CR = 3 between D2 and D7 with CR = 2 on D21 and CR = 1 on D24, and CC = 2 between D1 and D7 with CC = 1 on D21 and D24 in 1/3; CO = 4 between D3 and D7 and on D14 with CO = 2 on D21 and D24, CR = 3 between D2 and D7 with CR = 2 on D21 and CR = 1 on D24, and CC = 3 on D1 with CC = 1 on D21 and D24 in 1/3; CO = 4 between D3 and D14 with CO = 3 on D21 and CO = 2 on D24, CR = 3 between D1 and D7 with CR = 1 on D21 and D24, and CC = 2 between D1 and D2 and on D7 fully reversed by D21 in 1/3; CO = 4 between D3 and D4 with CO = 2 on D21 and D24, CR = 3 between D1 and D7 fully reversed by D17, and CC = 2 between D1 and D14 fully reversed by D17 in 1/3; CO = 4 between D3 and D14 with remaining scores unknown due to pannus formation, CR = 3 between D2 and D7 with CR = 2 on D21 and CR = 1 on D24, and CC = 2 between D1 and D7 with CC = 1 on D21 and D24 in 1/3; One animal sacrificed on D4 due to ruptured cornea with CO = 3 between D2 and D4, CR = 3 between D2 and D4, and CC = 2 on D1 with CC = 1 on D4	
4	bis-(3-Aminopropyl)-tetramethyldisiloxane	2469-55-8	Aliphatic Amine, primary| Disiloxane	L	Y	NICEATM	Alfa Aesar	97%	1 of 1	Cat 1	**CO mean ≥ 3**; IR mean > 1.5	2/2; 2/2	Unknown		CO = 4	2/2	Study terminated on D3; CO = 4 between Hr1 and D3 in 2/2	
5	Cyclohexanol	108-93-0	Alcohol| Cycloalkane	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	Cat 1	**CO mean ≥ 3**	3/4	CO pers D21	1/4			CO = 3 between D1 and D7 with CO = 1 on D21 in 1/4; CO = 3 between D2 and D3 fully reversed by D10 in 1/4; CO = 3 between D1 and D7 fully reversed by D14 in 1/4; CO = 3 between D1 and D3 fully reversed by D10 in 1/4	
6	Cyclohexyl isocyanate	3173-53-3	Cycloalkane| Isocyanate	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	Cat 1	**CO mean ≥ 3**	2/2	CO pers D21	2/2	CO = 4	2/2	CO = 4 between D1 and D21 in 2/2	
7	Diethylethanolamine (neat)	100-37-8	Alcohol| Aliphatic Amine, tertiary	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	Cat 1	**CO mean ≥ 3**	4/6	CO pers D21; Conj pers D21	5/6; 5/6	CO = 4	5/6	CO = 4 between D2 and D21, IR scores unknown, CR = 3 on D2 with CR = 1 on D21 and CC = 3 between D1 and D8 with CC = 1 on D21 in 1/6; CO = 4 on Hr1 and between D1 and D21, IR scores unknown, CR = 3 on D1 with CR = 1 on D21 and CC = 3 between D1 and D3 with CC = 2 on D21 in 1/6; CO = 4 between D8 and D21, IR = 1 between D1 and D2 with remaining scores unknown, CR = 2 between D1 and D14 with CR = 1 on D21 and CC = 3 between D3 and D14 with CC = 2 on D21 in 1/6; CO = 4 between D2 and D21, IR scores unknown, CR = 3 between D1 and D2 fully reversed by D14 and CC = 2 between D1 and D10 with CC = 1 on D21 in 1/6; CO = 4 between Hr1 and D21, IR scores unknown, CR = 3 between D1 and D2 fully reversed by D21 and CC = 3 between D1 and D14 with CC = 1 on D21 in 1/6; CO = 1 between D1 and D3 fully reversed by D8, IR = 1 between D1 and D8 fully reversed by D10, CR = 2 between D1 and D3 fully reversed by D21 and CC = 2 between D1 and D3 fully reversed by D8 in 1/6	
8	Diethylethanolamine (50%)	100-37-8	Alcohol| Aliphatic Amine, tertiary	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	Cat 1	**CO mean ≥ 3**	6/6	CO pers D21; Conj pers D21	6/6; 6/6	CO = 4	6/6	CO = 4 between D8 and D21, IR scores unknown, CR = 2 between D1 and D10 with CR = 1 on D21 and CC = 2 between D1 and D21 in 1/6; CO = 4 between Hr1 and D21, IR scores unknown, CR = 3 on D1 with CR = 1 on D21 and CC = 3 between D3 and D8 with CC = 2 on D21 in 1/6; CO = 4 between D8 and D21, IR scores unknown, CR = 3 on D1 with CR = 1 on D21 and CC = 3 on D8 with CC = 1 on D21 in 1/6; CO = 4 between Hr1 and D21, IR scores unknown, CR = 3 on D1 with CR = 1 on D21 and CC = 2 between D1 and D21 in 1/6; CO = 4 between Hr1 and Hr4 and between D2 and D21, IR scores unknown, CR = 3 on D1 with CR = 1 on D21 and CC = 3 between D10 and D14 with CC = 2 on D21 in 1/6; CO = 4 between Hr1 and D21, IR scores unknown, CR = 3 between D1 and D2 with CR = 1 on D21 and CC = 3 between D3 and D14 with CC = 2 on D21 in 1/6	
9	Diethylethanolamine (25%)	100-37-8	Alcohol| Aliphatic Amine, tertiary	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	Cat 1	**CO mean ≥ 3**	4/6	CO pers D21; Conj pers D21	6/6; 6/6	CO = 4	6/6	CO = 4 between D8 and D21, IR scores unknown, CR = 3 on D1 with CR = 1 on D21 and CC = 3 between D1 and D2 with CC = 2 on D21 in 1/6; CO = 4 between D8 and D21, IR = 1 between D1 and D2 with remaining scores unknown, CR = 2 between D1 and D10 with CR = 1 on D21 and CC = 3 between D10 and D14 with CC = 2 on D21 in 1/6; CO = 4 between D8 and D21, IR scores unknown, CR = 2 between D1 and D14 with CR = 1 on D21 and CC = 3 on D1 and D10 with CC = 1 on D21 in 1/6; CO = 4 between D8 and D21, IR = 1 between D1 and D2 with remaining scores unknown, CR = 2 between D1 and D10 with CR = 1 on D21 and CC = 2 between D1 and D14 with CC = 1 on D21 in 1/6; CO = 4 on D2 and between D8 and D21, IR scores unknown, CR = 2 between D1 and D14 fully reversed by D21 and CC = 2 between D1 and D14 with CC = 1 on D21 in 1/6; CO = 4 between D2 and D21, IR scores unknown, CR = 2 between D1 and D10 fully reversed by D21 and CC = 3 between D8 and D14 with CC = 1 on D21 in 1/6	
10	Ethylhexyl acid phosphate ester	12645-31-7	Alkoxy| Phosphate ester	L	Y	NICEATM	Merck	≥95%	1 of 1	Cat 1	**CO mean ≥ 3**	6/6	Unknown		CO = 4	6/6	Study terminated on D10 in 4/6 and on D7 in 2/6; CO = 4 between D2 and D10 in 2/6; CO = 4 between D1 and D2 and on D7 in 1/6; CO = 4 between D1 and D2 and between D7 and D10 in 1/6; CO = 4 on Hr1, between D2 and D3 and on D10 in 1/6; CO = 4 between D1 and D2 and on D7 in 1/6	
11	Lactic acid (neat)	50-21-5	Alcohol| Carboxylic acid	L	Y	NICEATM	Sigma-Aldrich	90%	1 of 1	Cat 1	**CO mean ≥ 3**	3/3	CO pers D21 (at least)	2/3	CO = 4	3/3	Study terminated on D14; CO = 4 between Hr1 and D13 fully reversed by D14 and IR = 2 between D2 and D8 fully reversed by D9 in 1/3; CO = 4 between Hr1 and D14 and IR = 2 between D5 and D14 in 1/3; CO = 4 between Hr1 and D14 and IR = 2 between D4 and D14 in 1/3; CR = 3 on D14 in 1/3; CR = 2 on D14 in 2/3; CC = 2 on D14 in 3/3; Delayed IR effects; Assumed CO irreversible	
12	Phosphorodicloridic acid, ethyl ester	1498-51-7	Alkoxy	L	Y	NICEATM	Sigma-Aldrich	96%	1 of 1	Cat 1	**CO mean ≥ 3**	6/6	CO pers D21 (at least)	6/6	CO = 4	6/6	Study terminated on D14; CO = 4 between Hr1 and D14 in 6/6; IR scores unknown; CR = 3 on D14 in 6/6; CC = 4 on D14 in 6/6; Assumed CO irreversible; A second study is also reported in NICEATM ALTTOX with the exact same animal scores and is considered a duplicate entry	
13	Pyridine (1 of 2)	110-86-1	Aryl| Pyridine	L	Y	ECETOC	Sigma-Aldrich	>99.9%	1 of 2	Cat 1	**CO mean ≥ 3**	2/3	CO pers D21 (at least)	at least 1/3	CO = 4	1/3	Study terminated on D14; Delayed effects; CO = 3 between D1 and D7 with CO = 4 on D14, IR = 2 between D2 and D14, CR = 3 between D1 and D14 and CC = 4 on D1 and D3 with CC = 3 on D14 in 1/3; CO = 2 between D1 and D7 with CO = 1 on D14, IR = 1 between D1 and D7 fully reversed by D14, CR = 3 between D2 and D7 with CR = 1 on D14 and CC = 4 on D3 with CC = 1 on D14 in 1/3; CO = 3 between D1 and D4 with CO = 2 on D14, IR = 1 between D1 and D4 fully reversed by D7, CR = 3 between D1 and D4 fully reversed by D14 and CC = 3 between D1 and D3 fully reversed by D14 in 1/3; Assumed CO irreversible	X
14	4-tert-Butylcatechol (85%, probably in methanol)	98-29-3	Precursors quinoid compounds| tert-Butyl	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	Cat 1	**CO mean ≥ 3**; IR mean > 1.5	6/6; 6/6	CO pers D21; Conj pers D21; IR pers D21	at least 4/6; at least 3/6; at least 3/6	CO = 4	6/6	Two animals sacrificed on D7 and 1 animal died on D20; CO = 4 between Hr1 and D21, IR = 2 between D1 and D7 and on D21, CR = 2 between D2 and D14 with CR = 1 on D21 and CC = 4 on D3 with CC = 2 on D21 in 1/6; CO = 4 between Hr1 and D21, IR = 2 between D1 and D7 with IR = 1 on D21, CR = 3 between D3 and D21 and CC = 4 between D3 and D7 with CC = 2 on D21 in 1/6; CO = 4 between Hr1 and D21, IR = 2 between D1 and D21, CR = 3 on D14 with CR = 2 on D21 and CC = 4 between D1 and D3 with CC = 3 on D21 in 1/6; CO = 4 between Hr1 and D14, IR = 2 between D1 and D14, CR = 2 between D1 and D14 and CC = 4 between D1 and D3 with CC = 3 on D14 in 1/6; CO = 4 between Hr1 and D7, IR = 2 between D1 and D7, CR = 2 on D1 and between D3 and D7 and CC = 4 on D1 and between D3 and D7 in 1/6; CO = 4 between Hr1 and D7, IR = 2 between D1 and D7, CR = 2 between D3 and D7 and CC = 4 between D3 and D7 in 1/6	
15	Aluminium chloride (concentration unknown)	16603-84-2	N/A	L (tested in solvent, available as S)	N	NICEATM	Unknown	Unknown	1 of 1	Cat 1	**CO mean ≥ 3**	4/6	CO pers D21; Conj pers D21	at least 5/6; at least 3/6	CO = 4	5/6	CO = 4 on D7 (score of D14 unknown) with CO = 2 on D21, CR = 3 on D14 with CR = 1 on D21 and CC = 3 between D1 and D2 with CC = 2 on D7 (scores of D14 and D21 unknown) in 1/6; CO = 4 between D1 and D7 (score of D14 unknown) with CO = 1 on D21, CR = 2 between D1 and D7 (scores of D14 and D21 unknown) and CC = 3 between D1 and D3 with CC = 2 on D7 (scores of D14 and D21 unknown) in 1/6; CO = 4 on D7 with CO = 2 on D21, CR = 2 between D2 and D14 with CR = 1 on D21 and CC = 3 on D1 with CC = 2 on D7 (scores of D14 and D21 unknown) in 1/6; CO = 2 between D2 and D3 with CO = 1 on D7 (scores of D14 and D21 unknown), CR = 2 between D1 and D14 with CR = 1 on D21 and CC = 2 between D1 and D7 fully reversed by D14 in 1/6; CO = 4 between D2 and D7 with CO = 2 on D21, CR = 2 between D1 and D7 (scores of D14 and D21 unknown) and CC = 3 on D1 and D3 with CC = 2 on D7 (scores of D14 and D21 unknown) in 1/6; CO = 4 on D7 with CO = 1 on D21, CR = 2 between D1 and D7 (scores of D14 and D21 unknown) and CC = 3 on D1 and D3 with CC = 2 on D7 (scores of D14 and D21 unknown) in 1/6	?
16	Benzalkonium chloride (10%)	63449-41-2	Ammonium salt| Benzyl	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	≥95%	1 of 1	Cat 1	**CO mean ≥ 3**; IR mean > 1.5	3/3; 3/3	CO pers D21; IR pers D21; Conj pers D21	3/3; 3/3; 2/3	CO = 4	3/3	CO = 4 between D1 and D21, IR = 2 between D1 and D21, CR = 3 between D3 and D7 with CR = 1 on D21 and CC = 4 between D1 and D3 with CC = 2 on D21 in 1/3; CO = 4 between D1 and D2 with CC = 2 on D21 in 1/3; CO = 4 between D2 and D21, IR = 2 between D1 and D21, CR = 3 between D1 and D7 fully reversed by D21 and CC = 4 between D1 and D3 with CC = 2 on D21 in 1/3; CO = 4 between D3 and D21, IR = 2 between D1 and D21, CR = 3 between D1 and D7 fully reversed by D21 and CC = 4 between D1 and D3 fully reversed by D21 in 1/3	
17	Benzethonium chloride (10%)	121-54-0	Alkane branched with quaternary carbon| Ammonium salt| Aryl| Benzyl| Ether| tert-Butyl	L (tested in solvent, available as S)	Y	LNS	Sigma-Aldrich	≥99%	1 of 1	Cat 1	**CO mean ≥ 3**	2/3	CO pers D21 (at least)	at least 2/3	CO = 4	2/3	Delayed effects; Irreversible lesions on D21 but scores unknown; CO = 3 between D2 and D7 with CO = 4 on D14 in 1/3; CO = 3 between D1 and D3 and on D7 with CO = 4 on D14 in 1/3; CO = 3 between D1 and D3 and on D14 in 1/3; IR = 1 on D14 in 3/3; CR and CC = 3 on D14 in 3/3	
18	Domiphen bromide (10%)	538-71-6	Ammonium salt| Aryl| Ether	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	97%	1 of 1	Cat 1	**CO mean ≥ 3**	2/3	CO pers D21 (at least)	at least 2/3	CO = 4	3/3	Study terminated on D14; Delayed effects; CO = 4 between D4 and D14 in 1/3; CO = 4 between D6 and D14 in 1/3; CO = 4 on D1 and between D3 and D7 with CO = 3 on D14 in 1/3; IR = 0 on D14 in 3/3; CR = 2 on D14 in 2/3; CR = 1 on D14 in 1/3; CC = 2 on D14 in 1/3; CC = 1 on D14 in 1/3; CC = 0 on D14 in 1/3; Assumed CO irreversible	
19	2-Benzyl-4-chlorophenol (1 of 2)	120-32-1	Aryl halide| Benzyl| Phenol	S	Y	NICEATM	Sigma-Aldrich	95%	1 of 2	Cat 1	**CO mean ≥ 3**	6/6	CO pers D21 (at least)	6/6	CO = 4	6/6	Study terminated on D16; CO = 4 between D1 and D16 in 6/6; IR scores unknown; CR = 3 on D16 in 6/6; CC = 3 on D16 in 2/6; CC = 2 on D16 in 4/6; Assumed CO irreversible	
20	2-Hydroxy iso-butyric acid	594-61-6	Alcohol| Carboxylic acid	S	Y	ZEBET	Sigma-Aldrich	99%	1 of 1	Cat 1	**CO mean ≥ 3**	3/3	Unknown		CO = 4	3/3	Study terminated on D3; CO = 4 between Hr1 and D3 in 2/3; CO = 4 between D1 and D3 in 1/3	
21	4,4'-(4,5,6,7-Tetrabromo-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromophenol] S,S-dioxide	4430-25-5	Aromatic perhalogencarbons| Aryl halide| Benzoxathiole S-oxide| Phenol| Sulfonate ester	S	Y	EURL ECVAM	Chemos GmbH	96.3%	1 of 1	Cat 1	**CO mean ≥ 3**	2/3	Unknown		CO = 4	1/3	Study terminated on D3; CO = 4 between D2 and D3 in 1/3	
22	4-[[2-Sulphatoethyl] sulphonyl]-aniline	2494-89-5	Aniline| Sulfate| Sulfone	S	Y	ZEBET	IS Chemical Technology	98%	1 of 1	Cat 1	**CO mean ≥ 3**	2/3	Unknown		CO = 4	2/3	Study terminated on D3; CO = 4 between Hr1 and D3 in 2/3	
23	4-(1,1,3,3-Tetramethylbutyl)phenol	140-66-9	Precursors quinoid compounds	S	Y	NICEATM	Sigma-Aldrich	97%	1 of 1	Cat 1	**CO mean ≥ 3**; IR mean > 1.5	6/6; 6/6	Unknown		CO = 4	1/6	Study terminated on D7; CO = 4 on D7 in 1/6	
24	alpha-Ketoglutaric acid	328-50-7	Carboxylic acid| Ketone| Oxocarboxylic acid	S	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 1	Cat 1	**CO mean ≥ 3**	3/3	Unknown		CO = 4	2/3	Study terminated on D3; CO = 4 on Hr1 and between D2 and D3 in 1/3; CO = 4 between D2 and D3 in 1/3	
25	Calcium thioglycolate (neat)	814-71-1	Carboxylic acid| Thioalcohol	S	Y	NICEATM	Sigma-Aldrich	≥98%	1 of 1	Cat 1	**CO mean ≥ 3**	3/3	CO pers D21 (at least)	3/3	CO = 4	3/3	Study terminated on D14; CO = 4 between Hr1 and D14 in 1/3; CO = 4 between D3 and D14 in 2/3; IR = 0 on D14 in 3/3; CR = 2 on D14 in 3/3; CC = 3 on D14 in 3/3; Assumed CO irreversible	

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
26	Dibenzoyl-L-tartaric acid (1 of 2)	2743-38-6	Aryl| Carboxylic acid| Carboxylic acid ester	S	Y	ECETOC	Sigma-Aldrich	98%	1 of 2	Cat 1	**CO mean ≥ 3**	2/3	Unknown				Study terminated on D14 with CO = 2, IR = 1, CC = 2 and CR = 2 in 1/3	
27	Dibenzoyl-L-tartaric acid (2 of 2)	2743-38-6	Aryl| Carboxylic acid| Carboxylic acid ester	S	Y	LNS	Sigma-Aldrich	98%	2 of 2	Cat 1	**CO mean ≥ 3**	2/3			CO = 4	2/3	CO = 4 between Hr1 and D4 in 2/3 fully reversed by D7 in 1/3 and by D21 in 1/3; Animal 1 with full reversibility of all endpoints on D7 (CO = 2 between D1 and D3 fully reversible by D4), animal 2 with full reversibility of all endpoints on D21 (CO = 4 between Hr1 and D4 fully reversible by D21) and animal 3 with full reversibility of all endpoints on D14 (CO = 4 between Hr1 and D4 fully reversible by D7)	
28	Distearyldimethylammonium chloride (neat)	107-64-2	Ammonium salt	S	Y	NICEATM	Sigma-Aldrich	≥97%	1 of 1	Cat 1	**CO mean ≥ 3**	3/3	CO pers D21 (at least)	3/3	CO = 4	3/3	Study terminated on D14; CO = 4 between D2 and D14 in 2/3; CO = 4 between D6 and D14 in 1/3; IR = 1 on D14 in 3/3; CR = 2 on D14 in 3/3; CC = 1 on D14 in 3/3; Assumed CO irreversible	
29	Ethyl lauroyl arginate HCl	60372-77-2	Aliphatic Amine, primary| Amidin| Carboxamide| Carboxylic acid ester| Guanidine	S	Y	EURL ECVAM	Proprietary	90.1%	1 of 1	Cat 1	**CO mean ≥ 3**	3/3	CO pers D21; Conj pers D21; IR pers D21	3/3; 3/3; at least 2/3	CO = 4	3/3	CO = 4 between Hr1 and D3 with CO = 3 on D21, IR scores unknown between Hr1 and D14 with IR = 2 on D21, CR = 3 between D1 and D3 with CR = 2 on D21 and CC = 4 between D1 and D3 with CC = 2 on D21 in 1/3; CO = 4 between Hr1 and D7 with CO = 3 on D21, IR scores unknown between Hr1 and D14 with IR = 2 on D21, CR = 3 between D1 and D7 with CR = 2 on D21 and CC = 4 between D1 and D14 with CC = 3 on D21 in 1/3; CO = 4 between Hr1 and D21, IR scores unknown between Hr1 and D21, CR = 3 between D1 and D7 with CR = 2 on D21 and CC = 4 between D1 and D7 with CC = 3 on D21 in 1/3	?
30	Imidazole (1 of 2)	288-32-4	Aryl| Imidazole	S	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 2	Cat 1	**CO mean ≥ 3**; IR mean > 1.5	3/3; 2/3	Possibly CO pers D21 (at least)	at least 2/3	CO = 4	2/3	Study terminated on D14; CO = 4 between D2 and D4 with CO = 2 on D14 in 1/3; CO = 4 between D2 and D3 with CO = 3 on D14 in 1/3; CO = 3 between D1 and D14 in 1/3; IR = 2 on D14 in 1/3; IR = 0 on D14 in 2/3; CR = 2 on D14 in 1/3; CR = 1 on D14 in 1/3; CR = 0 on D14 in 1/3; CC = 3 on D14 in 1/3; CC = 1 on D14 in 2/3	
31	Promethazine HCL (1 of 2)	58-33-3	Aliphatic Amine, tertiary| Phenothiazine	S	Y	ECETOC	Sigma-Aldrich	analytical grade	1 of 2	Cat 1	**CO mean ≥ 3**	3/3	Possibly CO pers D21 (at least)	3/3	CO = 4	3/3	Study terminated on D14; CO = 4 on Hr1 with CO = 3 on D14 in 3/3; IR = 0 on D14 in 3/3; CR = 1 on D14 in 2/3; CR = 0 on D14 in 1/3; CC = 1 on D14 in 2/3; CC = 0 on D14 in 1/3	
32	Promethazine HCL (2 of 2)	58-33-3	Aliphatic Amine, tertiary| Phenothiazine	S	Y	LNS	Sigma-Aldrich	analytical grade	2 of 2	Cat 1	**CO mean ≥ 3**	2/3	CO pers D21 (at least)	3/3	CO = 4	3/3	Delayed effects; Irreversible lesions on D21 but scores unknown; CO = 4 on Hr1 and D14 in 1/3; CO = 4 on Hr1 and between D7 and D14 in 1/3; CO = 4 on Hr1, D2 and D14 in 1/3; IR = 0 on D14 in 3/3; CR = 1 on D14 in 3/3; CC = 2 on D14 in 1/3; CC = 1 on D14 in 2/3	
33	Alkyl phosphoric acid ester/amine salt	Unknown	N/A	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	Cat 1	**CO mean ≥ 3**	6/6	Unknown		CO = 4	5/6	Study terminated on D7; CO = 4 between D1 and D3 and on D7 in 1/6; CO = 4 between D1 and D2 and on D7 in 1/6; CO = 4 between D1 and D7 in 2/6; CO = 4 between D3 and D7 in 1/6	?
34	Hydroxyethyl acrylate	818-61-1	Acrylate| Alcohol	L	Y	NICEATM	Sigma-Aldrich	96%	1 of 1	Cat 1	**IR mean > 1.5**	6/6	CO pers D21 (at least)	at least 4/6	CO = 4	4/6	Study terminated on D14; Delayed effects; Data missing for D2 in 6/6 but all 6 animals had IR = 2 on D1 and D3; CO = 4 between D3 and D14 in 2/6; CO =4 on D14 in 2/6; CO = 3 on D14 in 1/6; CO =2 between D3 and D14 in 1/6; IR = 2 on D14 in 6/6; CR = 3 on D14 in 4/6; CR = 2 on D14 in 2/6; CC = 4 on D14 in 5/6; CC = 1 on D14 in 1/6; Assumed CO irreversible	
35	Tetraethylene glycol diacrylate	17831-71-9	Acrylate| Ether	L	Y	NICEATM	Sigma-Aldrich	technical grade	1 of 1	Cat 1	**IR mean > 1.5**	6/6	CO pers D21 (at least)	at least 5/6	CO = 4	5/6	Study terminated on D14; Data missing for D2 in 6/6 and for IR on D1 in 1/6; All 6 animals had IR = 2 on D3 and 5/6 also had IR = 2 on D1; Delayed effects; CO = 4 between D3 and D14 in 2/6; CO = 4 between D7 and D14 in 3/6; CO = 3 on D3 with CO = 2 on D14 in 1/6; IR = 2 on D14 in 6/6; CR = 3 on D14 in 6/6; CC = 4 on D14 in 6/6; Assumed CO irreversible	
36	Triton X-100 (neat) (1 of 3)	9002-93-1	Alcohol| Alkane branched with quaternary carbon| Aryl| Ether| tert-Butyl	L	Y	NICEATM	Sigma-Aldrich	laboratory grade	1 of 3	Cat 1	**IR mean > 1.5**	5/6	Unknown				Study terminated on D7; CO = 2 on D7 in 2/6; CO = 1 on D7 in 4/6; IR = 1 on D7 in 6/6	
37	Triton X-100 (neat) (2 of 3)	9002-93-1	Alcohol| Alkane branched with quaternary carbon| Aryl| Ether| tert-Butyl	L	Y	NICEATM	Sigma-Aldrich	laboratory grade	2 of 3	Cat 1	**IR mean > 1.5**	4/6	Unknown		CO = 4	2/6	Study terminated on D7; Delayed effects; CO = 4 on D7 in 2/6; CO = 3 on D7 in 1/6; CO = 2 on D7 in 2/6; CO = 1 on D7 in 1/6; IR = 2 on D7 in 2/6; IR = 1 on D7 in 3/6; IR = 0 on D7 in 1/6	
38	Triton X-100/Magnesium carbonate (40%/60%)	Mixture (CAS: 9002-93-1; CAS: 546-93-0)	N/A	L	Y	NICEATM	Triton X-100: Sigma-Aldrich; Magnesium carbonate: Sigma-Aldrich	Triton X-100: laboratory grade; Magnesium carbonate: USP grade	1 of 1	Cat 1	**IR mean > 1.5**	4/6	Unknown		CO = 4	2/6	Study terminated on D7; Delayed effects; CO = 4 on D7 in 2/6; CO = 3 on D7 in 1/6; CO = 2 on D7 in 2/6; CO = 1 on D7 in 1/6; IR = 2 on D7 in 2/6; IR = 1 on D7 in 3/6; IR = 0 on D7 in 1/6 Triton X-100 is Triton X-120 of Triton X-100 series; all have same CASRN for Triton X-100	
39	Benzalkonium chloride (5%)	63449-41-2	Ammonium salt| Benzyl	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	≥95%	1 of 1	Cat 1	**IR mean > 1.5**	4/4	CO pers D21; Conj pers D21; IR pers D21	2/4; 1/4; 1/4	CO = 4	1/4	CO = 4 between D7 and D21, IR = 2 between D1 and D21, CR = 2 between D2 and D3 fully reversed by D21 and CC = 3 between D1 and D3 fully reversed by D21 in 1/4; CO = 3 between D1 and D3 with CO = 2 on D21, IR = 2 between D2 and D7 fully reversed by D14, CR = 2 between D1 and D10 with CR = 1 on D21 and CC = 3 between D1 and D2 with CC = 1 on D21 in 1/4; CO = 3 between D1 and D2 fully reversed by D10, IR = 2 between D1 and D3 fully reversed by D10, CR = 3 between D1 and D2 fully reversed by D21 and CC = 3 between D1 and D2 fully reversed by D10 in 1/4; CO = 3 between D1 and D2 fully reversed by D10, IR = 2 between D1 and D2 fully reversed by D7, CR = 2 between D1 and D3 fully reversed by D21 and CC = 3 between D1 and D3 fully reversed by D21 in 1/4	
40	Cetyl pyridinium bromide (10%)	140-72-7	Ammonium salt| Aryl| Pyridine	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	Cat 1	**IR mean > 1.5**; CO mean ≥ 3	6/6; 4/6	CO pers D21; Conj pers D21; IR pers D21	at least 4/6 (max 5); at least 3/6 (max 4); 3/6	CO = 4	2/6	CO = 4 between D2 and D21, IR = 2 between D1 and D14 with IR = 1 on D21, CR = 2 between D1 and D14 with CR = 1 on D21 and CC = 4 on D1 with CC = 1 on D21 in 1/6; CO = 4 between D14 and D21, IR = 2 between D1 and D14 with IR = 1 on D21, CR = 3 on D7 with CR = 2 on D21 and CC = 4 between D1 and D7 with CC = 2 on D21 in 1/6; CO = 3 between D1 and D21, IR = 2 between D1 and D7 with IR = 1 on D21, CR = 2 between D1 and D21 and CC = 4 between D1 and D3 with CC = 2 on D21 in 1/6; CO = 3 between D1 and D21, IR = 2 between D1 and D3 fully reversed by D14, CR = 2 between D1 and D7 fully reversed by D21 and CC = 4 between D1 and D2 fully reversed by D21 in 1/6; CO = 3 between D2 and D3 fully reversed by D10, IR = 2 between D1 and D2 fully reversed by D7, CR = 2 between D1 and D3 fully reversed by D14 and CC = 4 on D1 fully reversed by D7 in 1/6; Study terminated on D14 in 1/6: CO = 3 between D3 and D7 with CO = 1 on D14, IR = 2 between D1 and D7 fully reversed by D14, CR = 2 between D1 and D10 with CR = 1 on D14 and CC = 4 between D1 and D3 with CC = 1 on D14	
41	Cetyl pyridinium bromide (6%)	140-72-7	Ammonium salt| Aryl| Pyridine	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	Cat 1	**IR mean > 1.5**	3/4	Unknown				Study terminated on D10 for 1/4 with CO and IR = 1 and CR and CC = 2; Study terminated on D14 for 3/4 with CO = 1 in two animals and CR and CC = 1 in all three animals	
42	Antimony trioxide	1309-64-4	Carboxamide	S	Y	NICEATM	Sigma-Aldrich	99%	1 of 1	Cat 1	**IR mean > 1.5**	6/6	CO pers D21 (at least)	6/6	CO = 4	6/6	Study terminated on D14; Delayed effects; CO = 4 on D14 in 6/6; IR = 2 on D14 in 6/6; CR = 3 on D14 in 6/6; CC = 4 on D14 in 3/6; CC = 3 on D14 in 2/6; CC = 1 on D14 in 1/6; Assumed CO irreversible; A second study is also reported in NICEATM ALTTOX with the exact same animal scores and is considered a duplicate entry	
43	Benzothiazolium derivative	87699-86-3	N/A	S	N	NICEATM	Unknown	Unknown	1 of 1	Cat 1	**IR mean > 1.5**	3/3	Unknown				Study terminated on D2 due to irreversible iridic and conjunctival effects; CO = 0 in 3/3	?
44	Quinacrine (1 of 2)	69-05-6	Acridine| Aliphatic Amine, tertiary| Aryl halide| Ether	S	Y	ECETOC	Sigma-Aldrich	98%	1 of 2	Cat 1	**IR mean > 1.5**	2/3	Possibly CO pers D21 (at least)	3/3	CO = 4	3/3	Study terminated on D14 with CO = 3 in 3/3, IR = 2 in 3/3, and CR and CC = 2 in 3/3; CO = 4 on Hr1 in 3/3	
45	Xanthylium, 3,6-bis(diethylamino)-9-[2-(methoxy carbonyl)phenyl]-tetrafluoroborate	134429-57-5	Arene| Carboxylic acid ester| Conjugated hydrocarbon| Ether (cyclic)| Heterocyclic fragment| Imine	S	Y	EURL ECVAM	Proprietary	>99%	1 of 1	Cat 1	**IR mean > 1.5**	at least 2/3	Unknown		Other observations	3/3	Colour staining of cornea; Study terminated on D7	?
46	1,4-Dimethylbenzene	106-42-3	Aryl	L	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	Cat 1	CO > 0 **	** Conj 2/6	**CO pers D21** (at least)	1/6	CO = 4	1/6	Study terminated on D14 in 1/6; Delayed effects; CO = 4 between D7 and D14 (CO = 0 between D2 and D3), IR = 2 between D7 and D14, CR = 3 on D1 and between D3 and D14 and CC = 4 between D3 and D7 with CC = 1 on D14 in 1/6; CO and IR = 0 between Hr1 and D21 in 5/6; CR = 0 between D1 and D21 in 1/6; CR fully reversible by D2 in 1/6; CR fully reversible by D7 in 1/6; CR fully reversible by D14 in 2/6; CR fully reversible by D7 in 2/6; CR fully reversible by D14 in 2/6; CR fully reversible by D21 in 1/6; Assumed CO irreversible	X
47	1-Chloroctan-8-ol	23144-52-7	Alcohol| Alkyl halide	L	Y	ZEBET	Sigma-Aldrich	98%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	**CO pers D21**	3/3			CO = 1 between D1 and D21 in 3/3	
48	Acetic acid (10%)	64-19-7	Acetoxy| Carboxylic acid	L	Y	NICEATM	Sigma-Aldrich	≥99.7%	1 of 1	Cat 1	CO mean ≥ 1	3/3	**CO pers D21** (at least)	at least 2/3	CO = 4	2/3	Study terminated on D14; Delayed effects; CO = 4 on D14 in 2/3 and CO = 3 between D7 and D14 in 1/3; IR = 0 on D14 in 3/3; CR = 0 on D14 in 3/3; CC = 1 on D14 in 3/3; Assumed CO irreversible	
49	Benzyl alcohol (neat)	100-51-6	Alcohol| Benzyl	L	Y	NICEATM	Sigma-Aldrich	99.8%	1 of 1	Cat 1	CO mean ≥ 1	2/3	**CO pers D21** (at least)	at least 1/3	CO = 4	2/3	Study terminated on D14 in 2/3 and on D7 with full reversibility of all endpoints in 1/3; Delayed effects; CO = 4 between D10 and D14 in 1/3; CO = 4 between D8 and D12 with CO =3 on D14 in 1/3; CO = 1 between D3 and D4 fully reversed by D5 in 1/3; IR = 0 on D14 in 2/3; CR = 1 on D14 in 2/3; CC = 1 on D14 in 1/3; CC = 0 on D14 in 1/3; Assumed CO irreversible	
50	Bisphenol A, diethylene triamine, epichlorohydrin, polypropylene glycol diglycidyl ether, polymer (~60%, aqueous)	118569-52-1	Aliphatic Amine, primary| Aliphatic Amine, secondary| Alkyl halide| Epoxide| Ether| Phenol| Saturated heterocyclic fragment	L	Y	EURL ECVAM	Proprietary	~60%, aqueous	1 of 1	Cat 1	CO mean ≥ 3; IR mean > 1.5	1/1; 1/1	**CO pers D21**; Conj pers D21; IR pers D21	1/1; 1/1; 1/1			CO = 3 between D1 and D21, IR = 2 between D1 and D21 and CC = 3 on D1 with CC = 1 on D21 (CC = 0 between D7 and D14)	(X)/?
51	Butoxyethanol (1 of 3)	111-76-2	Alcohol| Alkoxy| Ether	L	Y	EURL ECVAM	Sigma-Aldrich	≥99%	1 of 3	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 5/6	**CO pers D21** (at least)	at least 1/6 (max 2)			CO = 1 between D1 and D3 with CO = 2 on D21 in 1/6; CO = 1 between D1 and D3 fully reversed by D7 in 3/6; CO = 2 on D3 fully reversed by D14 in 1/6; Study terminated on D14 for humane reasons after signs of discomfort with CO = 2 (CO = 1 between D1 and D3), IR = 1 (IR = 1 between D1 and D3) and CR and CC = 2 (CR and CC = 2 between D1 and D3) in 1/6; Scores between D1 and D3 almost identical in all 6 animals	X
52	Calcium sulphydrate (20% solution)	12133-28-7	N/A	L	N	ECETOC	Unknown	Unknown	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	1/1; 1/1	**CO pers D21**; Conj pers D21	1/1; 1/1			CO= 2 between D1 and D3 with CO = 1 on D21 in 1/1; CC = 4 between D1 and D3 with CC = 1 on D21 in 1/1	X
53	Coco alkyl dimethyl betaine (~30%, aqueous)	68424-94-2	Ammonium salt| Carboxylic acid	L	Y	EURL ECVAM	Proprietary	~30%, aqueous	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	4/4; 4/4	**CO pers D21**; Conj pers D21	4/4; 3/4			CO = 1 between D1 and D21 in 4/4; CR = 2 between D1 and D21 in 1/4; CR = 2 between D1 and D10 with CR = 1 on D21 in 1/4; CR = 3 between D1 and D3 with CR = 1 on D21 in 1/4; CR = 3 between D1 and D10 fully reversed by D21 in 1/4	?
54	Coco amidopropyl betaine (~30%, aqueous)	61789-40-0	Ammonium salt| Carboxamide| Carboxylic acid	L	Y	EURL ECVAM	Proprietary	~30%, aqueous	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	4/4; 4/4	**CO pers D21**; Conj pers D21	3/4; 2/4			CO = 1 between D1 and D21 and CR = 2 between D1 and D17 with CR = 1 on D21 in 1/4; CO = 1 between D1 and D21 and CR = 3 between D2 and D3 with CR = 1 on D21 in 1/4; CO = 1 between D1 and D21 and CR = 3 between D1 and D3 fully reversed by D21 in 1/4; CO = 1 between D1 and D3 fully reversed by D7 and CR = 3 between D2 and D3 fully reversed by D14 in 1/4; IR readings not reported	?
55	Di-sodium alkyl ether sulphosuccinate (~30%, aqueous)	68815-56-5	Alkoxy| Carboxylic acid| Ether| Sulfonic acid	L	Y	EURL ECVAM	Proprietary	~30%, aqueous	1 of 1	Cat 1	Conj mean ≥ 2; CO mean ≥ 1	4/4; 3/4	**CO pers D21**; Conj pers D21	1/4; 1/4			CO = 1 between D1 and D21 and CR = 3 between D2 and D3 with CR = 1 on D21 in 1/4; CO = 1 between D1 and D2 fully reversed by D3 and CR = 3 between D2 and D3 fully reversed by D10 in 1/4; CO = 1 between D1 and D3 fully reversed by D7 and CR = 3 on D2 fully reversed by D17 in 1/4; CO = 1 between D1 and D7 fully reversed by D10 and CR = 3 on D2 fully reversed by D10 in 1/4	X
56	EPIKOTE 604L	28768-32-3	Aromatic amine| Benzyl| Saturated heterocyclic fragment	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	Cat 1	CO mean ≥ 1	1/1	**CO pers D21**	1/1			CO = 2 between D2 and D3 with CO = 1 on D21 in 1/1	X
57	Ethanol (neat) (1 of 4)	64-17-5	Alcohol	L	Y	NICEATM	Sigma-Aldrich	>99.8%	1 of 4	Cat 1	Conj mean ≥ 2; CO mean ≥ 1; IR mean ≥ 1	6/6; 5/6; 5/6	**CO pers D21**	1/6			CO = 2 between D2 and D21 in 1/6; CO = 2 on D3 fully reversed by D7 in 1/6; CO = 2 on D2 fully reversed by D3 in 1/6; CO = 2 between D1 and D3 fully reversed by D7 in 1/6; CO = 2 between D2 and D7 fully reversed by D14 in 1/6; CO = 1 between D1 and D2 fully reversed by D3 in 1/6	X

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification: Severity		Drivers of Classification: Persistence		Drivers of Classification: Specific Observations		Comments	Should Not Be Used
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
58	Ethoxylated (5 EO) alkyl (C10-14) alcohol	66455-15-0	Alcohol| Alkoxy| Ether	L	Y	EURL ECVAM	Proprietary	90.5%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	**CO pers D21**	1/3			Delayed effects; CO = 1 between D1 and D6 increasing to CO = 3 on D8 until D21 in 1/3; CO = 2 between D2 and D8 fully reversed by D10 in 1/3; CO = 1 between D1 and D7 fully reversed by D8 in 1/3	X
59	Methyl cellosolve acetate	110-49-6	Acetoxy| Carboxylic acid ester| Ether	L	Y	NICEATM	Sigma-Aldrich	>98%	1 of 1	Cat 1	Conj mean ≥ 2	5/6	**CO pers D21**; Conj pers D21; IR pers D21	1/6; 1/6; 1/6			CO = 2 between D2 and D7 with CO = 2 on D21, IR = 1 between D1 and D21, CR = 3 between D2 and D21 and CC = 4 between D1 and D2 with CC = 2 on D21 in 1/6; CO = 0 between D1 and D21, IR = 1 on D1 fully reversed by D2, CR = 3 on D1 fully reversed by D7 and CC = 2 on D1 fully reversed by D7 in 1/6; CO = 0 between D1 and D21, IR = 0 between D1 and D21, CR = 2 on D1 fully reversed by D14 and CC = 1 on D1 fully reversed by D3 in 1/6; CO = 1 between D1 and D3 fully reversed by D7, IR = 1 between D1 and D3 fully reversed by D7, CR = 3 between D2 and D3 fully reversed by D7 and CC = 4 between D1 and D2 fully reversed by D7 in 1/6; CO = 1 between D1 and D2 fully reversed by D3, IR = 1 between D1 and D2 fully reversed by D3, CR = 3 between D1 and D2 fully reversed by D7 and CC = 3 between D1 and D2 fully reversed by D7 in 1/6; CO = 1 between D1 and D3 fully reversed by D7, IR = 1 between D1 and D2 fully reversed by D3, CR = 3 between D1 and D2 fully reversed by D14 and CC = 3 between D1 and D2 fully reversed by D7 in 1/6	X
60	Methyl pentynol	77-75-8	Alcohol| Alkyne	L	Y	ZEBET	Sigma-Aldrich	98%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	1/1; 1/1	**CO pers D21** (at least)	1/1	CO = 4	1/1	Study terminated on D14; Delayed effects; CO = 4 on D14 in 1/1; IR = 0 on D7 with unknown score on D14; CR and CC = 2 on D14 in 1/3; Assumed CO irreversible	X
61	Sodium alkyl ether sulphate (~27%, aqueous)	68891-38-3	Alkoxy| Ether| Sulfate	L	Y	EURL ECVAM	Proprietary	~27%, aqueous	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	4/4; 4/4	**CO pers D21**; Conj pers D21	2/4; 1/4			CO = 1 between D1 and D21 and CR = 3 between D1 and D10 with CR = 2 on D21 in 1/4; CO = 1 between D1 and D21 and CR = 3 between D1 and D3 fully reversed by D14 in 1/4; CO = 1 between D1 and D10 fully reversed by D14 and CR = 3 between D1 and D2 fully reversed by D17 in 1/4; CO = 1 between D1 and D7 fully reversed by D10 and CR = 3 on D2 fully reversed by D21 in 1/4	X
62	Sodium coco amphoacetate (~30%, aqueous)	61791-32-0	Alcohol| Aliphatic Amine, tertiary| Carboxamide| Carboxylic acid	L	Y	EURL ECVAM	Proprietary	~30%, aqueous	1 of 1	Cat 1	CO mean ≥ 1	3/4	**CO pers D21**; Conj pers D21	1/4; 1/4			CO = 1 between D1 and D21 and CR = 2 between D1 and D3 and between D14 and D17 with CR = 1 on D21 in 1/4; CO = 1 on D1 fully reversed by D2 and CR = 2 on D2 fully reversed by D3 in 1/4; CO = 1 between D1 and D3 fully reversed by D7 and CR = 2 between D1 and D2 fully reversed by D10 in 1/4; CO = 1 between D1 and D14 fully reversed by D17 and CR = 3 between D2 and D3 fully reversed by D17 in 1/4	X
63	Surfonic HDL-1 (Chemical name: Nonyl phenol ethoxylate, branched)	9016-45-9	Alcohol| Benzyl| Ether	L	Y	NICEATM	Unknown	Unknown	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 6/6	**CO pers D21** (at least)	at least 4/6 (max 5)	CO = 4	5/6	Study terminated on D14; Delayed effects; CO = 4 on D14 in 3/6; CO = 4 between D7 and D14 in 1/6; CO = 4 between D3 and D7 fully reversed by D14 in 1/6; CO = 3 between D1 and D7 with CO = 2 on D14; IR = 1 on D14 in 2/6; IR = 2 on D7 with unknown score on D14 in 1/6; IR = 0 on D14 in 3/6; CR = 2 on D14 in 3/6; CR = 1 on D14 in 3/6; CC = 3 on D14 in 1/6; CC = 2 on D14 in 4/6; CC = 1 on D14 in 1/6; Assumed CO irreversible	?
64	Surfonic N-102 (Chemical name: Nonyl phenol ethoxylate, branched)	9016-45-9	Alcohol| Benzyl| Ether	L	Y	NICEATM	Unknown	Unknown	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 6/6	**CO pers D21** (at least)	at least 2/6 (max 4)	CO = 4	2/6	Study terminated on D14; Delayed effects; CO = 4 on D14 in 2/6; CO = 2 between D1 and D7 fully reversed by D14 in 1/6; CO = 2 between D1 and D7 in 1/6 with animal dying on D11 for reasons unrelated to the test chemical; CO = 2 between D1 and D3 fully reversed by D7 with unknown score on D14 in 1/6; CO = 3 on D7 with unknown score on D14; IR = 1 on D14 in 1/6; IR = 0 on D14 in 4/6; CR = 1 on D14 in 5/6; CC = 3 on D14 in 1/6; CC = 2 on D14 in 4/6; Assumed CO irreversible	?
65	Triethanol ammonium alkyl sulphate (~40%, aqueous)	90583-18-9	Alcohol| Aliphatic Amine, tertiary| Alkoxy| Sulfate	L	Y	EURL ECVAM	Proprietary	~40%, aqueous	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	4/4; 4/4	**CO pers D21**; Conj pers D21	1/4; 1/4			CO = 1 between D1 and D21 and CR = 3 between D1 and D3 with CR = 1 on D21 in 1/4; CO = 1 between D1 and D3 fully reversed by D7 and CR = 3 between D1 and D3 fully reversed by D14 in 1/4; CO = 1 between D1 and D3 fully reversed by D7 and CR = 3 between D1 and D2 fully reversed by D14 in 1/4; CO = 1 between D1 and D7 fully reversed by D10 and CR = 3 between D1 and D2 fully reversed by D14 in 1/4	X
66	Benzalkonium chloride (1%) (1 of 2)	63449-41-2	Ammonium salt| Benzyl	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	≥95%	1 of 2	Cat 1	Conj mean ≥ 2	3/4	**CO pers D21**; Conj pers D21	1/4; 1/4			Delayed effects; CO = 3 on D7 with CO = 1 on D21 and CR and CC = 2 between D2 and D7 with CR and CC = 1 on D21 in 1/4; CO = 2 on D2 fully reversed by D7, CR = 2 between D1 and D2 fully reversed by D10 and CC = 3 on D1 fully reversed by D10 in 1/4; CO = 1 between D1 and D2 fully reversed by D3, CR = 2 on D1 fully reversed by D7 and CC = 2 between D1 and D2 fully reversed by D7 in 1/4; CO = 1 on D1 fully reversed by D2, CR = 2 on D1 fully reversed by D10 and CC = 3 on D1 fully reversed by D10 in 1/4	X
67	Benzalkonium chloride (1%) (2 of 2)	63449-41-2	Ammonium salt| Benzyl	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	≥95%	2 of 2	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 6/6	**CO pers D21**; Conj pers D21	at least 2/6 (max 3); at least 2/6 (max 3)	CO = 4	1/6	Delayed effects; CO = 4 on D14 with CO = 3 on D21, CC = 3 between D1 and D3 with CC = 1 on D21 in 1/6; CO = 3 on D3 with CO = 2 on D21, CC = 4 on D1 fully reversed by D14 in 1/6; CO = 2 between D1 and D14 fully reversed by D21, CC = 3 between D1 and D3 with CC = 1 on D21 in 1/6; CO =2 between D1 and D10, CC = 4 between D1 and D2 with CC = 2 on D10, study terminated on D10 in 1/6; CO = 2 between D1 and D7 fully reversed by D10, CC = 3 on D1 fully reversed by D10 in 1/6; CO = 2 between D1 and D3 fully reversed by D7, CC = 3 between D1 and D2 fully reversed by D10 in 1/6	X
68	Cetylpyridinium chloride (10%)	6004-24-6	Ammonium salt| Aryl| Pyridine	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	>99%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**CO pers D21** (at least)	at least 2/3	CO = 4	3/3	Study terminated on D14; CO = 4 between D7 and D14 in 1/3; CO = 4 between D1 and D14 in 1/3; CO = 4 between D1 and D13 with CO = 3 on D14 in 1/3; IR = 1 on D14 in 3/3; CR = 2 on D14 in 2/3; CR = 1 on D14 in 1/3; CC = 2 on D14 in 1/3; CC = 1 on D14 in 2/3; Assumed CO irreversible	
69	Cetyltrimethyl ammonium bromide (CTAB) (10%) (1 of 2)	57-09-0	Ammonium salt	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 2	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 2/3; 2/3	**CO pers D21** (at least)	3/3	CO = 4	3/3	Study terminated on D14; Delayed effects; CO = 4 between D10 and D14 in 2/3; CO = 4 between D8 and D14 in 1/3; IR = 0 on D14 in 3/3; CR = 3 on D14 in 1/3; CR = 2 on D14 in 2/3; CC = 2 on D14 in 3/3; Assumed CO irreversible	
70	Cetyltrimethyl ammonium bromide (CTAB) (10%) (Hexadecyltrimethylammonium bromide reported in LNS) (2 of 2)	57-09-0	Ammonium salt	L (tested in solvent, available as S)	Y	LNS	Sigma-Aldrich	≥99%	2 of 2	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**CO pers D21** (at least)	at least 1/3	CO = 4	1/3	Delayed effects; Persistent corneal lesions; Irreversible lesions on D21 but scores unknown; CO = 4 on D14 in 1/3; CO = 3 between D7 and D14 in 1/3; CO = 3 on D14 in 1/3; IR = 1 on D14 in 2/3; IR = 0 on D14 in 1/3; CR and CC = 3 on D14 in 1/3; CR and CC = 2 on D14 in 2/3	
71	Di(2-ethylhexyl)sodium sulphosuccinate (10%)	577-11-7	Alkane, branched with tertiary carbon| Carboxylic acid ester| Sulfonic acid	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 2/3	**CO pers D21** (at least)	at least 1/3 (max 2)	CO = 4	1/3	Delayed effects; Study terminated on D14; CO = 4 on D14 in 1/3; CO = 3 between D3 and D6 with CO = 1 on D14 in 1/3; CO = 2 between D1 and D9 fully reversed by D12 in 1/3; IR = 0 on D14 in 3/3; CR and CC = 1 on D14 in 1/3; CR and CC = 0 on D14 in 2/3; Assumed CO irreversible	
72	Potassium laurate (10%)	10124-65-9	Carboxylic acid	L (tested in solvent, available as S)	Y	NICEATM	MP Biomedicals	90-100%	1 of 1	Cat 1	CO > 0 **	** CO 1/3; Conj 1/3; IR 1/3	**CO pers D21** (at least)	1/3	CO = 4	1/3	Study terminated on D14 in 1/3 and on D7 with full reversibility of all endpoints in 2/3; Delayed effects; CO = 4 between D7 and D14 in 1/3; CO = 0 between D1 and D7 in 1/3; CO = 1 between D1 and D2 fully reversed by D3 in 1/3; IR = 0 on D14 in 1/3; CR = 2 on D14 in 1/3; CC = 1 on D14 in 1/3; Assumed CO irreversible	X
73	Sodium hydroxide (10%)	1310-73-2	Hydrazine	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	≥98%	1 of 1	Cat 1	CO mean ≥ 3; IR mean > 1.5	1/1; 1/1	**CO pers D21**; Conj pers D21; IR pers D21	1/1; 1/1; 1/1	CO = 4	1/1	CO = 4 between D1 and D21, IR = 2 between D1 and D21 and CR and CC = 3 between D1 and D21 in 1/1	(X)
74	Sodium lauryl sulphate (10%) (1 of 3)	151-21-3	Alkoxy| Sulfate	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 3	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 2/3; 2/3	**CO pers D21** (at least)	3/3	CO = 4	3/3	Study terminated on D14; Delayed effects; CO = 4 between D7 and D14 in 2/3; CO = 4 between D5 and D14 in 1/3; IR = 1 on D14 in 2/3; IR = 0 on D14 in 1/3; CR = 3 on D14 in 1/3; CR = 1 on D14 in 2/3; CC = 2 on D14 in 1/3; CC = 1 on D14 in 1/3; CC = 0 on D14 in 1/3; Assumed CO irreversible	X
75	Sodium lauryl sulphate (10%) (2 of 3)	151-21-3	Alkoxy| Sulfate	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99%	2 of 3	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	2/3; 2/3	**CO pers D21** (at least)	at least 1/3 (max 2)	CO = 4	1/3	Study terminated on D14 in 2/3 and on D7 with full reversibility of all endpoints in 1/3; Delayed effects; CO = 4 between D5 and D14 in 1/3; CO = 3 between D3 and D14 in 1/3; CO = 1 between D1 and D2 fully reversed by D3 in 1/3; IR = 0 on D14 in 2/3; CR and CC = 2 on D14 in 1/3; CR and CC = 1 on D14 in 1/3; Assumed CO irreversible	X
76	Sodium lauryl sulphate (15%)	151-21-3	Alkoxy| Sulfate	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 5/6; 4/6	**CO pers D21**	1/6			CO = 2 on D1 with CO = 1 on D21 in 1/6; CO = 2 between D1 and D2 fully reversed by D7 in 3/6; CO = 2 between D1 and D3 fully reversed by D7 in 1/6; CO = 2 on D1 fully reversed by D7 in 1/6	X
77	Stearyltrimethylammonium chloride (10%)	112-03-8	Ammonium salt	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥95%	1 of 1	Cat 1	CO mean ≥ 1; IR mean ≥ 1; Conj mean ≥ 2	3/3; 3/3; 2/3	**CO pers D21** (at least)	3/3	CO = 4	3/3	Study terminated on D14; Delayed effects; CO = 4 between D2 and D14 in 1/3; CO = 4 between D6 and D14 in 1/3; CO = 4 between D12 and D14 in 1/3; IR = 1 on D14 in 1/3; IR = 0 on D14 in 2/3; CR = 3 on D14 in 1/3; CR = 2 on D14 in 2/3; CC = 2 on D14 in 2/3; CC = 1 on D14 in 1/3; Assumed CO irreversible	
78	Trichloroacetic acid (30%)	76-03-9	Alkyl halide| Carboxylic acid	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	>99%	1 of 1	Cat 1	CO mean ≥ 3; IR mean > 1.5	1/1; 1/1	**CO pers D21**; Conj pers D21; IR pers D21	1/1; 1/1; 1/1	CO = 4	1/1	CO = 4 between D1 and D3 with CO = 2 on D21, IR = 2 between D1 and D21, CR = 2 between D1 and D7 with CR = 2 on D21 and CC = 3 between D1 and D3 with CC = 2 on D21 in 1/1	(X)
79	1,2-Dihydro-1,3,4,6-tetramethyl-2-oxo-pyrimidinium hydrogensulphate	54424-29-2	Aliphatic Amine, tertiary| Allyl| Unsaturated heterocyclic amine| Unsaturated heterocyclic fragment	S	Y	EURL ECVAM	Proprietary	89.4%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3	**CO pers D21**; IR pers D21	2/3; 1/3			CO = 3 between D3 and D14 with CO = 2 on D21 and IR = 1 between D1 and D21 in 1/3; CO = 1 between D1 and D21 and IR = 0 between D1 and D21 in 1/3; CO = 3 on D1 fully reversed by D7 and IR = 1 between D1 and D3 fully reversed by D7 in 1/3	?
80	1-Naphthalene acetic acid	86-87-3	Benzyl| Carboxylic acid| Fused carbocyclic aromatic| Naphtalene	S	Y	ECETOC	Sigma-Aldrich	>95%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	6/6; 4/6	**CO pers D21**; Conj pers D21; IR pers D21	1/6; 1/6; 1/6	CO = 4	1/6	Delayed effects; CO = 4 between D14 and D21, IR = 2 between D2 and D3 with IR = 1 on D21, CR = 2 between D1 and D3 and between D10 and D21 and CC = 2 between D2 and D3 and between D10 and D21 in 1/6; CO = 2 on D1 fully reversed by D7, IR = 1 on D1 and D3 fully reversed by D7, CR = 2 on D1 fully reversed by D7 and CC = 1 on D1 fully reversed by D2 in 1/6; CO = 1 between D1 and D10 fully reversed by D14, IR = 1 on D1 fully reversed by D2, CR = 2 on D1 fully reversed by D7 and CC = 1 on D1 fully reversed by D2 in 1/6; CO = 1 between D1 and D7 fully reversed by D10, IR = 1 on D1 fully reversed by D2, CR = 2 between D1 and D3 fully reversed by D10 and CC = 1 between D1 and D3 fully reversed by D7 in 1/6; CO = 2 on D1 fully reversed by D21, IR = 2 between D2 and D3 fully reversed by D10, CR = 2 between D1 and D3 fully reversed by D14 and CC = 2 on D1 fully reversed by D7 in 1/6; CO = 2 between D1 and D3 fully reversed by D10, IR = 1 between D1 and D3 fully reversed by D7, CR = 3 on D1 fully reversed by D10 and CC = 1 between D1 and D3 fully reversed by D7 in 1/6	X
81	1-Naphthalene acetic acid Na salt	61-31-4	Benzyl| Carboxylic acid| Fused carbocyclic aromatic| Naphtalene	S	Y	ECETOC	TCI	≥99%	1 of 1	Cat 1	CO mean ≥ 1; IR mean ≥ 1; Conj mean ≥ 2	6/6; 6/6; 4/6	**CO pers D21**; Conj pers D21; IR pers D21	4/6; 4/6; 1/6	CO = 4	1/6	CO = 4 between D1 and D21, IR = 2 between D1 and D21, CR = 2 on D14 with CR = 1 on D21 and CC = 4 between D1 and D2 with CC = 3 on D21 in 1/6; CO = 3 between D1 and D14 with CO = 1 on D21, IR = 1 between D1 and D10 fully reversed by D14, CR = 2 between D1 and D10 with CR = 1 on D21 and CC = 2 between D2 and D3 and between D10 and D14 with CC = 1 on D21 in 1/6; CO = 3 on D1 and between D7 and D10 with CO = 2 on D21, IR = 1 between D1 and D7 fully reversed by D10, CR = 3 on D1 with CR = 1 on D21 and CC = 3 on D1 with CC = 2 on D21 in 1/6; CO = 3 between D2 and D21, IR = 1 between D1 and D7 fully reversed by D10, CR = 1 between D1 and D21 and CC = 2 between D1 and D2 and between D7 and D21 in 1/6; CO = 1 between D1 and D10 fully reversed by D14, IR = 1 between D1 and D7 fully reversed by D10, CR = 2 between D1 and D3 fully reversed by D10 and CC = 2 between D1 and D3 fully reversed by D7 in 1/6; CO = 1 between D1 and D3 fully reversed by D7, IR = 1 between D1 and D7 fully reversed by D10, CR = 2 between D1 and D3 fully reversed by D7 and CC = 1 between D1 and D3 fully reversed by D7 in 1/6	X
82	2,7-Naphthalenediol	582-17-2	Fused carbocyclic aromatic| Naphtalene| Phenol	S	Y	EURL ECVAM	Sigma-Aldrich	97%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	1/1; 1/1; 1/1	**CO pers D21**; Conj pers D21	1/1; 1/1			CO = 2 between D1 and D14 with CO = 1 on D21 and CR = 3 between D2 and D3 with CR = 1 on D21 in 1/1	X
83	2-[(4-Amino-2-nitrophenyl)amino]benzoic acid	117907-43-4	Aniline| Aryl| Carboxylic acid| Nitrobenzene	S	Y	Cosmetics Europe	Proprietary	Unknown	1 of 1	Cat 1	CO > 0 **	** CO 2/4; Conj 2/4	**CO pers D21**; Conj pers D21	1/4; 1/4			CO = 1 between D1 and D21 and CR = 2 between D1 and D14 with CR = 1 on D21 in 1/4; CO = 1 and CR = 2 between D1 and D3 fully reversed by D7 in 1/4; CO = 0 between D1 and D21 and CR = 1 between D1 and D2 fully reversed by D3 in 1/4; CO = 0 between D1 and D21 and CR = 1 on D1 fully reversed by D2 in 1/4; IR effects not numerically recorded but the study report states that no IR effects were detected	X

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
84	2-Benzyl-4-chlorophenol (2 of 2)	120-32-1	Aryl halide| Benzyl| Phenol	S	Y	NICEATM	Sigma-Aldrich	95%	2 of 2	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 6/6	**CO pers D21**; Conj pers D21; IR pers D21	5/6; 5/6; at least 5/6	CO = 4	1/6	Delayed effects; CO = 4 between D4 and D21, IR = 1 between D1 and D3 with remaining scores unknown, CR = 3 between D1 and D21 and CC = 4 between D2 and D21 in 1/6; CO = 3 between D10 and D19 with CO = 2 on D21, IR = 2 between D4 and D14 with IR = 1 on D21, CR = 3 between D2 and D7 with CR = 2 on D21 and CC = 4 between D3 and D4 with CC = 1 on D21 in 1/6; CO = 3 on D4 and between D16 and D21, IR = 2 on D4 with IR = 1 on D21, CR = 3 between D1 and D10 and on D21 and CC = 4 between D2 and D4 with CC = 1 on D21 in 1/6; CO = 3 on D4 and D10 with CO = 1 on D21, IR = 2 between D4 and D14 with IR = 1 on D21, CR = 3 between D1 and D4 fully reversed by D16 and CC = 4 between D2 and D4 fully reversed by D19 in 1/6; CO = 2 between D1 and D16 fully reversed by D21, IR = 2 on D7 with IR = 1 on D21, CR = 3 between D1 and D14 with CR = 2 on D21 and CC = 4 between D3 and D4 with CC = 1 on D21 in 1/6; CO = 3 between D2 and D13 with CO = 2 on D21, IR = 2 between D4 and D14 with IR = 1 on D21, CR = 3 between D1 and D21 and CC = 4 between D3 and D4 and on D10 with CC = 1 on D21 in 1/6	
85	2-Methylresorcinol	608-25-3	Precursors quinoid compounds	S	Y	EURL ECVAM	Sigma-Aldrich	98%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	1/1; 1/1; 1/1	**CO pers D21**; Conj pers D21	1/1; 1/1			CO = 3 between D1 and D2 with CO = 1 on D21 and CR = 3 between D1 and D7 with CR = 2 on D21 in 1/1	X
86	3,4-Dichlorophenyl isocyanate	102-36-3	Aryl halide| Isocyanate	S	Y	NICEATM	Sigma-Aldrich	97%	1 of 1	Cat 1	Conj mean ≥ 2	2/3	**CO pers D21**	3/3			Delayed effects; CO = 2 on D7 with CO = 1 on D21 in 1/3; CO = 1 between D7 and D21 in 1/3; CO = 1 between D2 and D21 in 1/3	
87	Acid Red 92 (Chemical name: 3,4,5,6-Tetrachloro-2-(1,4,5,8-tetrabromo-6-hydroxy-3-oxoxanthen-9-yl)-benzoic acid) (neat)	18472-87-2	Aromatic perhalogencarbons| Aryl halide| Fused carbocyclic aromatic| Fused saturated heterocycles| Heterocyclic spiro rings| Isobenzofuran| Lactone| Phenol| Xanthene	S	Y	NICEATM	Sigma-Aldrich	≥80%	1 of 1	Cat 1	CO mean ≥ 1	3/3	**CO pers D21** (at least)	at least 2/3	CO = 4	3/3	Study terminated on D14; Delayed effects; CO = 4 between D10 and D14 in 1/3; CO = 4 between D4 and D14 in 1/3; CO = 4 between D6 and D8 with CO = 3 on D14 in 1/3; IR = 0 on D14 in 3/3; CR = 2 on D14 in 1/3; CR = 1 on D14 in 2/3; CC = 2 on D14 in 1/3; CC = 1 on D14 in 1/3; CC = 0 on D14 in 1/3; Assumed CO irreversible	
88	Captan 90-concentrate	133-06-2	Alkyl halide| Allyl| Sulfen amide| Tetrahydrophthalimide	S	Y	ECETOC	TCI	>98%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**CO pers D21**; Conj pers D21; IR pers D21	3/3; 2/3; 1/3	CO = 4	3/3	Delayed effects; CO = 4 between D3 and D21, IR = 2 between D10 and D21, CR = 3 between D1 and D21 and CC = 4 on D1 and D3 with CC = 1 on D21 in 1/3; CO = 4 between D2 and D3 with CO = 2 on D21, IR = 1 between D1 and D3 fully reversed by D7, CR = 3 between D1 and D7 fully reversed by D15 and CC = 3 between D1 and D2 fully reversed by D15 in 1/3; CO = 4 between D7 and D10 with CO = 3 on D21, IR = 2 on D10 fully reversed by D15, CR = 3 between D1 and D10 with CR = 1 on D21 and CC = 3 between D1 and D3 fully reversed by D21 in 1/3	
89	Imidazole (2 of 2)	288-32-4	Aryl| Imidazole	S	Y	LNS	Sigma-Aldrich	≥99%	2 of 2	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**CO pers D21** (at least)	at least 1/3			Delayed effects; Irreversible lesions on D21 but scores unknown; CO = 2 between D1 and D14 in 1/3; CO = 3 on D14 in 2/3; IR = 0 on D14 in 3/3; CR = 2 on D14 in 2/3; CR = 0 on D14 in 1/3; CC = 2 on D14 in 3/3	
90	Lauric acid	143-07-7	Carboxylic acid	S	Y	ECETOC	Sigma-Aldrich	>99%	1 of 1	Cat 1	Conj mean ≥ 2; CO mean ≥ 1	3/3; 2/3	**CO pers D21**; Conj pers D21	3/3; 3/3			CO = 2 between D7 and D21 and CR = 3 between D1 and D7 with CR = 1 on D21 in 1/3; CO = 2 between D7 and D21 and CR = 3 between D1 and D2 with CR = 1 on D21 in 1/3; CO = 2 between D7 and D14 with CO = 1 on D21 and CR = 3 between D1 and D7 with CR = 1 on D21 in 1/3	
91	m-Phenylene diamine (neat)	108-45-2	Aminoaniline, meta	S	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3	**CO pers D21** (at least)	3/3	CO = 4	3/3	Study terminated on D14; Delayed effects; CO = 4 between D1 and D14 in 1/3 (CO = 3 on D13); CO = 4 between D11 and D14 in 1/3; CO = 4 between D9 and D14 in 1/3; IR = 0 on D14 in 3/3; CR = 2 on D14 in 1/3; CR = 1 on D14 in 2/3; CC = 1 on D14 in 2/3; CC = 0 on D14 in 1/3; Assumed CO irreversible	
92	N-(2-Amino-4,6-dichloropyrimidin-5-yl) formamide	171887-03-9	Aromatic heterocyclic halide| Aryl halide| Formylamino	S	Y	EURL ECVAM	Chemos GmbH	99.5%	1 of 1	Cat 1	CO > 0 **	** CO 2/4; IR 2/4; Conj 1/4	**CO pers D21**	1/4			CO = 2 between D2 and D3 with CO = 1 on D21 in 1/4; CO = 0 between D1 and D3 in 2/4; CO = 1 between D1 and D3 fully reversed by D7 in 1/4	X
93	Pinoxaden	243973-20-8	Carboxylic acid ester| Ether (cyclic)| Heterocyclic fragment| Hydrazide| Lactam	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	**CO pers D21**; Conj pers D21	1/3; 1/3			Delayed effect; CO = 3 on D17 with CO = 2 on D21 fully reversed by D28, CR = 2 on D3 with CR = 1 on D21 and CC = 3 between D1 and D3 with CC = 1 on D21 in 1/3; CO = 1 between D1 and D7 fully reversed on D10, CR = 2 on D3 fully reversed by D17 and CC = 3 between D1 and D2 fully reversed by D7 in 1/3; CO = 1 between D1 and D3 fully reversed on D7, CR = 1 between D1 and D7 fully reversed by D10 and CC = 3 on D1 fully reversed by D7 in 1/3	X
94	p-tert-Butylphenol (neat) (10 mg)	98-54-4	Phenol| tert-Butyl	S	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	Cat 1	CO mean ≥ 1; IR mean ≥ 1	6/6; 4/6	**CO pers D21**; Conj pers D21	4/6; 1/6	CO = 4	1/6	Delayed effects; 10 mg dose; CO = 4 between D14 and D21, IR = 1 between D1 and D3 with remaining scores unknown, CR = 2 on D14 with CR = 1 on D21 and CC = 2 between D1 and D2 and on D14 with CC = 1 on D21 in 1/6; CO = 3 on D3 with CO = 1 on D21, IR = 1 between D1 and D3 fully reversed by D7, CR = 1 between D1 and D3 fully reversed by D7 and CC = 2 between D1 and D3 fully reversed by D14 in 1/6; CO = 2 between D1 and D7 with CO = 1 on D21, IR = 1 between D1 and D3 fully reversed by D7, CR = 1 between D1 and D3 fully reversed by D7 and CC = 2 on D1 fully reversed by D7 in 1/6; CO = 2 between D1 and D7 with CO = 1 on D21, IR = 1 between D1 and D3 fully reversed by D7, CR = 2 on D3 fully reversed by D7 and CC = 1 between D1 and D3 fully reversed by D7 in 1/6; CO = 2 on D1 and D3 fully reversed by D14, IR = 1 between D1 and D3 fully reversed by D7, CR = 1 between D1 and D3 fully reversed by D7 and CC = 3 on D1 fully reversed by D7 in 1/6; CO = 1 between D1 and D7 fully reversed by D14, IR = 1 on D1 fully reversed by D2, CR = 1 between D1 and D3 fully reversed by D7 and CC = 2 on D1 fully reversed by D7 in 1/6	
95	p-tert-Butylphenol (neat) (80 mg)	98-54-4	Phenol| tert-Butyl	S	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	6/6; 6/6	**CO pers D21**; Conj pers D21	5/6; 1/6	CO = 4	4/6	Delayed effects; 80 mg dose; CO = 4 between D7 and D21, IR scores unknown and CC = 4 on D1 with CC = 1 on D21 in 1/6; CO = 4 between D7 and D14 with CO = 3 on D21, IR = 1 on D1 with remaining scores unknown and CC = 4 on D1 and D3 fully reversed by D21 in 1/6; CO = 4 between D7 and D14 with CO = 3 on D21, IR scores unknown and CC = 4 on D1 and D3 fully reversed by D21 in 1/6; CO = 4 between D7 and D14 with CO = 3 on D21, IR scores unknown and CC = 4 on D1 and D3 fully reversed by D21 in 1/6; CO = 3 between D1 and D2 with CO = 2 on D21, IR scores unknown between D1 and D14 but fully reversed by D21 and CC = 4 on D1 and D3 fully reversed by D14 in 1/6; CO = 2 between D1 and D3 fully reversed by D14, IR = 1 between D1 and D3 fully reversed by D7 and CC = 4 on D1 and D3 fully reversed by D14 in 1/6	
96	Quinacrine (2 of 2)	69-05-6	Acridine| Aliphatic Amine, tertiary| Aryl halide| Ether	S	Y	LNS	Sigma-Aldrich	98%	2 of 2	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**CO pers D21**; IR pers D21 (at least)	at least 1/3; at least 1/3	CO = 4	2/3	Delayed and persistent IR effects; Irreversible lesions on D21 but scores unknown; CO = 4 between Hr1 and D1 with CO = 3 on D14 and IR = 2 on D14 in 1/3; CO = 4 on Hr1 with CO = 3 on D14 and IR = 2 on D14 in 1/3; CO = 2 between D1 and D14 and IR = 2 on D14 in 1/3; CR and CC =2 on D14 in 3/3	
97	Soap from 80/20 tallow/coconut oil	Mixture	N/A	S	Y	ECETOC	Unknown	Unknown	1 of 1	Cat 1	Conj mean ≥ 2	3/3	**CO pers D21**; Conj pers D21	1/3; 1/3			Very slight opacity (0.5) between D1 and D14 with CO = 1 on D21 and CR = 3 between D1 and D7 with CR = 1 on D21 in 1/3; Very slight opacity (0.5) between D1 and D14 fully reversed by D21 and CR = 3 between D1 and D3 fully reversed by D14 in 1/3; Very slight opacity (0.5) between D1 and D14 fully reversed by D21 and CR = 3 between D2 and D3 fully reversed by D14 in 1/3	X
98	Sodium oxalate (1 of 2)	62-76-0	Oxocarboxylic acid	S	Y	LNS	Sigma-Aldrich	≥99.5%	1 of 2	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**CO pers D21** (at least)	1/3	CO = 4	1/3	Irreversible lesions on D21 in 1/3 but scores unknown; CO = 4 between D3 and D14 irreversible on D21 (score unknown), IR = 1 between D1 and D7 fully reversed by D14, CR = 3 between D1 and D7 with CR = 2 on D14 and CC = 4 between D1 and D7 with CC = 2 on D14 in 1/3; CO = 2 between D1 and D7 fully reversed by D14, IR = 1 between D1 and D4 fully reversed by D7, CR = 3 between D1 and D4 with CR = 1 on D14 and CC = 4 on D1 and between D3 and D4 with CC = 1 on D14 in 1/3; CO = 2 between D1 and D7 fully reversed by D14, IR = 1 between D1 and D3 fully reversed by D4, CR = 3 between D1 and D4 fully reversed by D14 and CC = 4 between D1 and D4 fully reversed by D14 in 1/3	X
99	Sodium oxalate (2 of 2)	62-76-0	Oxocarboxylic acid	S	Y	ECETOC	Sigma-Aldrich	≥99.5%	2 of 2	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**CO pers D21** (at least)	at least 1/3 (max 2)	CO = 4	1/3	Study terminated on D14; Delayed effects; CO = 4 between D7 and D14, IR = 2 between D2 and D3 and on D14, CR = 3 between D1 and D14 and CC = 4 between D1 and D3 with CC = 3 on D14 in 1/3; CO = 3 between D3 and D7 with CO = 2 on D14, IR = 1 between D1 and D7 fully reversed by D14, CR = 3 between D1 and D7 fully reversed by D14 and CC = 4 between D1 and D3 fully reversed by D14 in 1/3; CO = 2 between D1 and D7 fully reversed by D14, IR = 1 between D1 and D3 fully reversed by D4, CR = 3 between D1 and D4 fully reversed by D14 and CC = 3 on D2 fully reversed by D14 in 1/3; Assumed CO irreversible	X
100	Sodium perborate tetrahydrate	10486-00-7	N/A	S	Y	ECETOC	Sigma-Aldrich	≥97%	1 of 1	Cat 1	Conj mean ≥ 2; CO mean ≥ 1; IR mean ≥ 1	6/6; 5/6; 4/6	**CO pers D21**; Conj pers D21	4/6; 2/6	CO = 4	2/6	Delayed effects; CO = 4 between D14 and D21 and CR = 3 between D1 and D7 with CR = 1 on D21 in 1/6; CO = 4 on D21 and CR = 3 between D1 and D7 fully reversed by D21 in 1/6; CO = 2 between D1 and D7 with CO = 1 on D21 and CR = 3 between D1 and D7 fully reversed by D21 in 1/6; CO = 2 between D2 and D14 with CO = 1 on D21 and CR = 3 between D1 and D7 with CR = 1 on D21 in 1/6; CO = 2 between D1 and D3 fully reversed by D14 and CR = 3 between D1 and D3 fully reversed by D21 in 1/6; CO = 0 between D1 and D21 and CR = 3 between D1 and D3 fully reversed by D14 in 1/6	
101	Sodium salicylate (neat)	54-21-7	Carboxylic acid| Phenol	S	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	**CO pers D21** (at least)	at least 2/3	CO = 4	3/3	Study terminated on D14; CO = 4 between D4 and D14 in 2/3; CO = 4 between Hr1 and D13 with CO = 3 on D14 in 1/3; IR = 0 on D14 in 3/3; CR = 2 on D14 in 2/3; CR = 0 on D14 in 1/3; CC = 2 on D14 in 2/3; CC = 1 on D14 in 1/3; Assumed CO irreversible	
102	3,6-Dimethyloctanol	151-19-9	Alcohol| Alkane, branched with tertiary carbon	Unknown	N	ZEBET	Sigma-Aldrich	Unknown	1 of 1	Cat 1	CO mean ≥ 1	3/3	**CO pers D21**; Conj pers D21	1/3; 1/3			CO = 1 between D1 and D14 with CO = 2 on D21 and CR = 2 between D1 and D3 with CR = 1 on D21 in 1/3; CO = 1 between D1 and D3 fully reversed by D7 and CR = 2 between D1 and D2 fully reversed by D7 in 1/3; CO = 1 between D1 and D3 fully reversed by D7 and CR = 1 between D1 and D3 fully reversed by D7 in 1/3	X
103	7-Acetoxyheptanal	29425-54-5	Acetoxy| Aldehyde| Carboxylic acid ester	Unknown	N	ZEBET	Unknown	Unknown	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	**CO pers D21**; Conj pers D21	1/3; 1/3			Delayed effects; CO = 3 between D14 and D21, CR = 2 between D1 and D21 and CC = 2 on D1, D3 and D14 with CC = 1 on D21 in 1/3; CO = 1 between D1 and D3 fully reversed by D7, CR = 3 between D1 and D3 fully reversed by D14 and CC = 2 between D1 and D3 fully reversed by D7 in 1/3; CO = 1 between D1 and D7 fully reversed by D14, CR = 2 between D1 and D3 fully reversed by D7 and CC = 2 between D1 and D3 fully reversed by D7 in 1/3	X
104	AU-358 LTV	Proprietary to Sewer Sciences Inc.	N/A	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3	**CO pers D21**	3/3	CO = 4	1/3	CO = 4 between D7 and D10 with CO = 1 on D21 in 1/3; CO = 1 between D1 and D21 in 2/3	?
105	C12/C14-Glucoside	Unknown	N/A	Unknown	N	ZEBET	Unknown	Unknown	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	**CO pers D21**; Conj pers D21	3/3; 3/3			CO = 2 between D7 and D21, CR = 2 between D1 and D21 and CC = 2 between D1 and D14 with CC = 1 on D21 in 1/3; CO = 2 on D3 and D21, CR = 2 between D1 and D7 with CR = 2 on D21 and CC = 2 between D1 and D3 with CC = 2 on D21 in 1/3; CO = 2 on D21, CR = 2 between D1 and D3 with CR = 2 on D21 and CC = 1 between D1 and D3 fully reversed by D7	?
106	Diphocars	154836-02-9	N/A	Unknown	N	ZEBET	Unknown	Unknown	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	1/1; 1/1; 1/1	**CO pers D21** (at least)	1/1	CO = 4	1/1	Study terminated on D14; Delayed effects; CO = 4, IR = 2, CR = 3 and CC = 1 on D14 in 1/1; Assumed CO irreversible	X
107	Polyhexamethylene guanidine	31961-54-3	Guanidine	Unknown	N	ZEBET	Unknown	Unknown	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 2/3	**CO pers D21**; Conj pers D21	1/3; 1/3	CO = 4	1/3	Delayed effects; CO = 4 on D21, IR = 1 between D1 and D4 with IR = 0 on D14 and scores on D7 and D21 unknown, CR = 3 between D2 and D7 with CR = 2 on D21 and CC = 2 between D1 and D14 with CC = 1 on D21 in 1/3; CO = 2 between D3 and D4 fully reversed by D14, IR = 1 between D3 and D7 fully reversed by D14, CR = 1 between D1 and D7 fully reversed by D14 and CC = 1 between D1 and D7 fully reversed by D14 in 1/3; CO = 1 between D1 and D7 fully reversed by D14, IR = 1 between D1 and D4 fully reversed by at least D14 (score on D7 unknown), CR = 3 between D2 and D7 fully reversed by D14 and CC = 2 on D2 and between D4 and D7 fully reversed by D14 in 1/3	X
108	(Ethylenediamine propyl)trimethoxysilane	1760-24-3	Aliphatic Amine, primary| Aliphatic Amine, secondary| AlkoxySilane	L	Y	EURL ECVAM	Sigma-Aldrich	≥80%	1 of 1	Cat 1	Conj mean ≥ 2; IR mean ≥ 1; CO mean ≥ 1	3/3; 3/3; 2/3	**Conj pers D21**; CO pers D21	3/3; 2/3			CO = 2 on D4 with CO = 1 on D21, CR = 3 on D1 with CR = 1 on D21 and CC = 3 on D1 fully reversed by D14 in 1/3; CO = 1 between D1 and D21, CR = 3 on D1 with CR = 1 on D21 and CC = 2 between D1 and D4 fully reversed by D7 in 1/3; CO = 3 on D7 fully reversed by D21, CR = 3 between D2 and D7 with CR = 1 on D21 and CC = 2 between D1 and D7 with CC = 1 on D21 in 1/3	

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
109	Alkyl (C10-16) glucoside (~50%, aqueous)	110615-47-9	Dihydroxyl group	L	Y	EURL ECVAM	Proprietary	~50%, aqueous	1 of 1	Cat 1	CO > 0 **	** CO 2/4; Conj 2/4	**Conj pers D21**; CO pers D21	2/4; 1/4			CO = 1 between D1 and D21, CR = 3 between D1 and D2 with CR = 1 on D21 and CC = 2 between D1 and D2 with CC = 1 on D21 in 1/4; CO = 1 between D1 and D17 fully reversed by D21, CR = 3 on D1 (scores of D2 and D3 unknown) with CR = 1 on D21 and CC = 2 on D1 (score of D2 unknown) fully reversed by D21 in 1/4; CO = 0 between D1 and D21, CR = 2 on D1 fully reversed by D10 and CC = 1 between D1 and D2 fully reversed by D3 in 1/4; CO = 0 between D1 and D21, CR = 2 on D1 fully reversed by at least D7 (score of D3 unknown) and CC = 1 between D1 and D2 fully reversed by at least D7 (score of D3 unknown) in 1/4	
110	Butoxyethanol (Butyl cellosolve reported in ECETOC) (2 of 3)	111-76-2	Alcohol| Alkoxy| Ether	L	Y	ECETOC	Sigma-Aldrich	≥99%	2 of 3	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**Conj pers D21**	3/3			CR = 3 between D1 and D3 with CR = 1 on D21 and CC = 3 between D1 and D3 fully reversed by D14 in 1/3; CR = 2 between D1 and D3 with CR = 1 on D21 and CC = 3 between D1 and D3 fully reversed by D21 in 1/3; CR = 2 between D1 and D7 fully reversed by D21 and CC = 3 on D1 with CC = 1 on D21 in 1/3	X
111	Protectol PP	80-54-6	Aldehyde| Benzyl| tert-Butyl	L	Y	NICEATM	Sigma-Aldrich	analytical standard	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	**Conj pers D21**; CO pers D21	3/3; 2/3			CO = 1 between D1 and D21 and CR = 2 between D1 and D21 in 1/3; CO = 2 between D8 and D17 with CO = 1 on D21 and CR = 3 between D17 and D21 in 1/3; CO = 1 between D1 and D3 fully reversed by D8 and CR = 2 between D1 and D3 with CR = 1 on D21	
112	Triton X-100 (10%)	9002-93-1	Alcohol| Alkane branched with quaternary carbon| Aryl| Ether| tert-Butyl	L	Y	ECETOC	Sigma-Aldrich	laboratory grade	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 6/6	**Conj pers D21**	1/6			CR = 2 between D1 and D3 with CR = 1 on D21 in 1/6; CR = 2 between D1 and D3 fully reversed by D10 in 1/6; CR = 2 between D1 and D3 fully reversed by D14 in 4/6	X
113	Igepon AC-78 (10%) (Chemical name: Sodium cocoyl isethionate)	58969-27-0 (original CAS # deleted and replaced by 61789-32-0)	Carboxylic acid ester| Sulfonic acid	L (tested in solvent, neat chemical unknown)	Y	ECETOC	Unknown	Unknown	1 of 1	Cat 1	CO mean ≥ 1	6/6	**Conj pers D21**	1/6			CR = 3 on D1 with CR = 1 on D21 in 1/6; CR = 2 between D1 and D2 fully reversed by D10 in 2/6; CR = 2 on D1 fully reversed by D14 in 1/6; CR = 2 on D1 fully reversed by D7 in 1/6; CR = 3 on D1 fully reversed by D10 in 1/6	X
114	2,5-Dimethylhexanediol	110-03-2	Dihydroxyl group	S	Y	ECETOC / ZEBET	Sigma-Aldrich	97%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	**Conj pers D21**; IR pers D21	1/3; 1/3			IR = 1 between D1 and D21, CR = 3 between D1 and D3 with CR = 2 on D21 and CC = 3 between D1 and D2 with CC = 1 on D21 in 1/3; IR = 0 between D1 and D21, CR = 2 between D1 and D3 fully reversed by D15 and CC = 2 between D1 and D2 fully reversed by D8 in 1/3; IR = 0 between D1 and D21, CR = 2 between D1 and D3 fully reversed by D15 and CC = 2 on D1 fully reversed by D8; Two studies are reported in ECETOC and ZEBET with the exact same animal scores and are considered duplicate entries	X
115	2-[(4-Aminophenyl)azo]-1,3-dimethyl-1H-imidazolium chloride	97404-02-9	Ammonium salt| Aniline| Aryl| Azo| Guanidine| Imidazole	S	Y	EURL ECVAM	Sigma-Aldrich	93.4%	1 of 1	Cat 1	Conj mean ≥ 2; IR mean ≥ 1; CO mean ≥ 1	3/3; 3/3; 2/3	**Conj pers D21** (at least)	at least 1/3			CR = 3 between D2 and D4 with CR = 1 on D21 in 1/3; CR = 3 between D2 and D4 (study terminated on D4) in 2/3	X
116	3,4-Dimethyl-1H-pyrazole	2820-37-3	Allyl| Aryl| Pyrazole	S	Y	EURL ECVAM	Sigma-Aldrich	≥97%	1 of 1	Cat 1	CO mean ≥ 1; IR mean ≥ 1; Conj mean ≥ 2	3/3; 3/3; 2/3	**Conj pers D21**; CO pers D21; IR pers D21	3/3; 2/3; 2/3			CO = 3 between D14 and D21, IR = 2 between D7 and D21 and CR = 2 on D7 with CR = 1 on D21 in 1/3; CO = 2 between D1 and D21, IR = 2 between D1 and D7 with IR = 2 on D21 and CR = 2 on D7 with CR = 1 on D21 in 1/3; CO = 1 between D1 and D7 fully reversed by D14, IR = 1 between D1 and D14 fully reversed by D21 and CR = 2 between D1 and D7 with CR = 1 on D21 in 1/3	
117	5,6-Dihydroxyindoline HBr	138937-28-7	Indoline| Precursors quinoid compounds	S	Y	EURL ECVAM	Chemos GmbH	99.7%	1 of 1	Cat 1	Conj mean ≥ 2; IR mean ≥ 1	3/3; 2/3	**Conj pers D21**	2/3			CR = 3 between D1 and D21 in 2/3; CR = 3 between D1 and D7 fully reversed by D21 in 1/3	
118	5-Chloro-2-(4-chlorophenoxy)phenol	3380-30-1	Arene| Aryl halide| Phenol	S	Y	EURL ECVAM	Proprietary	Unknown	1 of 1	Cat 1	Conj mean ≥ 2	2/3	**Conj pers D21**; CO pers D21	2/3; 1/3			CO = 1 between D2 and D21 and CR = 1 between D1 and D21 in 1/3; CO = 1 between D2 and D7 fully reversed by D14 and CR = 2 between D1 and D3 with CR = 1 on D21 in 1/3; CO = 0 between D1 and D21 and CR = 2 between D1 and D3 fully reversed by D14 in 1/3	X
119	Aminopyralid	150114-71-9	Aromatic heterocyclic halide| Aryl halide| Carboxylic acid	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3	**Conj pers D21**; CO pers D21	3/3; 1/3	Other observations	3/3	CO = 2 between D1 and D21, CR = 3 on D3 with CR = 2 on D21 and CC = 3 between D1 and D3 with CC = 2 on D21 in 1/3; CO = 2 between D1 and D14 fully reversed by D21, CR = 3 on D1 with CR = 1 on D21 and CC = 2 on D1 fully reversed by D21 in 1/3; CO = 2 on D1 fully reversed by D21, CR = 3 between D1 and D7 with CR = 1 on D21 and CC = 3 on D1 fully reversed by D21 in 1/3; Pannus formation in 3/3 reversible in at least 2/3	X
120	Benzoic acid	65-85-0	Aryl| Carboxylic acid	S	Y	EURL ECVAM	Sigma-Aldrich	≥99.5%	1 of 1	Cat 1	Conj mean ≥ 2; CO mean ≥ 1	3/3; 2/3	**Conj pers D21**; CO pers D21	3/3; 2/3			CO = 3 between D1 and D3 with CO = 2 on D21, IR = 2 on D14 with sore on D21 unknown, CR = 3 between D1 and D21 and CC = 2 between D1 and D2 and on D7 with CC = 1 on D21 in 1/3; CO = 1 between D1 and D21, IR = 1 on D2 fully reversed by D3, CR = 3 between D1 and D21 and CC = 2 between D1 and D7 with CC = 1 on D21 in 1/3; CO = 1 between D2 and D3 fully reversed by D7, IR = 0 between D1 and D21, CR = 3 between D1 and D7 with CR = 1 on D21 and CC = 2 on D1 and D3 fully reversed by D14 in 1/3	
121	Disodium 2,2'-([1,1'-biphenyl]-4,4'-diyldivinylene) bis(benzene sulphonate)	27344-41-8	Alkene| Aryl| Biphenyl| Sulfonic acid	S	Y	EURL ECVAM	TCI	>97%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	**Conj pers D21**	2/3			CR = 2 between D1 and D3 with CR = 1 on D21 in 1/3; CR = 2 between D1 and D7 with CR = 1 on D21 in 1/3; CR = 2 between D1 and D3 fully reversed by D14 in 1/3	X
122	Soap from 80/20 palm oil/coconut oil	Mixture	N/A	S	Y	ECETOC	Unknown	Unknown	1 of 1	Cat 1	Conj mean ≥ 2; CO mean ≥ 1	3/3; 2/3	**Conj pers D21**	2/3			CR = 3 between D1 and D2 with CR = 1 on D21 in 2/3; CR = 3 between D2 and D3 fully reversed by D21 in 1/3	X
123	(3-Aminopropyl)triethoxy silane (1 of 2)	919-30-2	Aliphatic Amine, primary| Alkoxy| Alkoxysilane	L	Y	NICEATM	Sigma-Aldrich	99%	1 of 2	Cat 1	NA		Unknown		**CO = 4**	2/3	Study terminated on D1	
124	(3-Aminopropyl)triethoxy silane (2 of 2)	919-30-2	Aliphatic Amine, primary| Alkoxy| Alkoxysilane	L	Y	NICEATM	Sigma-Aldrich	99%	2 of 2	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; at least 5/6	Unknown		**CO = 4**	6/6	Delayed effects; Study terminated on D7 with CO = 4 in 5/6 and CO = 2 in 1/6; CO = 4 on D7 in 3/6, between Hr1 and D7 in 1/6, between D2 and D7 in 1/6 and between Hr1 and H4 in 1/6	
125	Methoxyethyl acrylate	3121-61-7	Acrylate| Ether	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	Cat 1	Conj mean ≥ 2; CO mean ≥ 1	3/3; 2/3	Unknown		**CO = 4**	2/3	CO = 4 on D1 in 2/3 fully reversed by D3 in 1/3; Study terminated for the other animal on D14 with CO = 1	X
126	Methyl thioglycolate	2365-48-2	Carboxylic acid ester| Thioalcohol	L	Y	ECETOC	Sigma-Aldrich	95%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3			**CO = 4**	1/3	CO = 4 between Hr1 and D1 in 1/3 fully reversed by D10; Animal 1 with full reversibility of all endpoints on D6 (CO on D3, max CO = 3), animal 2 on D7 (CO on D7, max CO = 3) and animal 3 on D10 (CO on D10, max CO = 4)	X
127	n-Butanol (10%)	71-36-3	Alcohol	L	Y	NICEATM	Sigma-Aldrich	99.8%	1 of 1	Cat 1	CO mean ≥ 1	2/3	Unknown		**CO = 4**	1/3	Study terminated on D14 with CO = 1 in 1/3; CO = 4 in this animal between D3 and D9, which reduces to score 1 on D13; No corneal effects on one of the other animals and CO = 1 in the last animal fully reversed by D5	X
128	n-Butanol (neat) (1 of 2)	71-36-3	Alcohol	L	Y	ZEBET	Sigma-Aldrich	99.8%	1 of 2	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; at least 2/3	Unknown		**CO = 4**	1/3	Study terminated on D7 with CO = 4 in 1/3; CO = 4 between D2 and D7	X
129	n-Octylamine	111-86-4	Aliphatic Amine, primary	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	Cat 1	NA		Unknown		**CO = 4**	4/4	Study terminated on D1	
130	Polyethylene glycol 400, dichloride	27252-69-3	N/A	L	Y	NICEATM	Unknown	Unknown	1 of 1	Cat 1	Conj mean ≥ 2; IR mean ≥ 1; CO mean ≥ 1	6/6; 5/6; 4/6	Unknown		**CO = 4**	4/6	Delayed effects; Study terminated on D7 with CO = 4 in 4/6; CO = 4 on D7 in 4/6	?
131	tert-Butyl hydroperoxide (70%, aqueous)	75-91-2	Aliphatic hydroperoxide| tert-Butyl	L	Y	NICEATM	Sigma-Aldrich	70%, aqueous	1 of 1	Cat 1	CO mean ≥ 1	6/6	Unknown		**CO = 4**	1/6	Delayed effects; Study terminated on D7 with CO = 4 in 1/6, CO = 3 in 3/6 and CO = 2 in 2/6; CO = 4 on D7 in 1/6	X
132	Tetrahydrofuran	109-99-9	Oxolane| Saturated heterocyclic fraement	L	Y	NICEATM	Sigma-Aldrich	≥99.9%	1 of 1	Cat 1	CO mean ≥ 1; IR mean ≥ 1; Conj mean ≥ 2	6/6; 6/6; 5/6	Unknown		**CO = 4**	2/6	Delayed effects; Study terminated on D7 with CO = 4 in 2/6; CO = 4 between D4 and D7 in 2/6	X
133	Tributyltin oxide	56-35-9	Stannoxane	L	Y	NICEATM	Sigma-Aldrich	96%	1 of 1	Cat 1	NA		Unknown		**CO = 4**	4/6	Study terminated on D3 with CO = 4 in 4/6; CO = 1 in 1/6 and CO unknown in 1/6; CO = 4 on D3 in 4/6; No CO data reported for D1 to D3 in 1/6 and for D1 to D2 in 2/6 (obscured)	
134	Trichloroacetyl chloride	76-02-8	Acyl halide| Perhaloeenated carbons derivatives	L	Y	NICEATM	Sigma-Aldrich	99%	1 of 1	Cat 1	NA		Unknown		**CO = 4**	4/4	Study terminated on D7 with CO = 4 in 4/4; Data missing between D2 and D4; CO = 4 between Hr1 and D7 in 4/4	
135	Acid Red 92 (Chemical name: 3,4,5,6-Tetrachloro-2-(3,4,5,8-tetrabromo-6-hydroxy-3-oxoxanthen-9-yl)-benzoic acid) (10%)	18472-87-2	Aromatic perhalogencarbons| Aryl halide| Fused carbocyclic aromatic| Fused saturated heterocycles| Heterocyclic spiro rings| Isobenzofuran| Lactone| Phenol| Xanthene	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥80%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	2/3; 2/3	Unknown		**CO = 4**	1/3	Study terminated on D14 with CO = 1 in 1/3; CO = 4 in this animal between D9 and D11, which reduces to score 1 on D12	X
136	Sodium undecylenate solution (33.2%, aqueous)	3398-33-2	Allyl| Carboxylic acid	L (tested in solvent, available as S)	Y	ECETOC	SCBT	90-100%	1 of 1	Cat 1	CO mean ≥ 3	1/1			**CO = 4**	1/1	CO = 4 between D1 and D3 in 1/1 fully reversed by D11; Study terminated on D11 with CO, IR, CR and CC = 0	X
137	(-)-trans-4-(4'-Fluorophenyl)-3-hydroxymethyl-1-methyl piperidine	105812-81-5	Alcohol| Alkane, branched with tertiary carbon| Aryl halide| Piperidine| Saturated heterocyclic amine| Saturated heterocyclic fragment	S	Y	EURL ECVAM	Chemos GmbH	98.5%	1 of 1	Cat 1	NA		Unknown		**CO = 4**	1/3	Study terminated on D2 with CO = 4, IR = 1, CR = 3 and CC = 4 in 1/3; CO = 2, IR = 1, CR and CC = 3 in 1/3; CO = 2, IR = 1, CR = 3 and CC = 4 in 1/3	X
138	1,2,4-Triazole Na salt	41253-21-8	Aryl| Triazole	S	Y	ECETOC	Sigma-Aldrich	90%	1 of 1	Cat 1	CO mean ≥ 3; IR mean > 1.5	1/1; 1/1	Unknown		**CO = 4**	1/1	CO = 4 between Hr1 and D3; Study terminated on D3 with CO = 4, IR = 2, CR = 3 and CC = 3	X
139	1,2-Benzisothiazol-3(2H)-one	2634-33-5	Benzothiazole/ Benzoisothiazole	S	Y	EURL ECVAM	Chemos GmbH	99.8%	1 of 1	Cat 1	NA		Unknown		**CO = 4**	4/6	Study terminated on D2; CO = 4 on D2 in 4/6	
140	1,3-Diiminobenz (f)-isoindoline	65558-69-2	Fused carbocyclic aromatic| Iminoisoindole| Iminolactams| Naphtalene	S	Y	NICEATM	Sigma-Aldrich	95%	1 of 1	Cat 1	NA		Unknown		**CO = 4**	4/4	Study terminated on D7 with CO = 4 in 4/4; Data only for D1 and D7; CO = 4 between D1 and D7 in 2/4 and on D7 in 2/4	
141	3-Amino-2,4-dichlorophenol HCl	61693-43-4	Aniline| Aryl halide| Phenol	S	Y	EURL ECVAM	Unknown	Unknown	1 of 1	Cat 1	NA		Unknown		**CO = 4**	1/1	Study terminated on D1 with CO = 4 in 1/1	X
142	4-Amino-5-methoxy-2-methylbenzene-sulphonic acid	6471-78-9	Aniline| Ether| Sulfonic acid	S	Y	ZEBET	SCBT	96%	1 of 1	Cat 1	CO mean ≥ 3	1/1	Unknown		**CO = 4**	1/1	Study terminated on D3 with CO = 4 in 1/1; CO = 4 between D1 and D3	X
143	4-Chloro-methanilic acid	98-36-2	Aniline| Aryl halide| Sulfonic acid	S	Y	ZEBET	TCI	>98%	1 of 1	Cat 1	CO mean ≥ 3	1/1	Unknown		**CO = 4**	1/1	Delayed effects; Study terminated on D7 with CO = 4 in 1/1; CO = 4 on D7	X
144	Acid blue 40 (Chemical name: 1-Amino-4-[4-(acetylamino)anilino]-9,10-dioxoanthracene-2-sulfonic acid monosodium salt)	6424-85-7	Aniline| Anthracenone/ Antracendione| Aryl| Carboxamide| Sulfonic acid	S	Y	NICEATM	SCBT	100%	1 of 1	Cat 1	Conj mean ≥ 2; CO mean ≥ 1	5/6; 4/6	Unknown		**CO = 4**	2/6	Study terminated on D14 with CO = 2 in 1/6 and CO = 0 in 5/6; CO = 4 on D1 in 1/6 (reduced to CO = 2 on D14) and between D2 and D3 in 1/6 (fully reversed by D14); CO = 0 between Hr1 and D14 in 2/6	X
145	Benzalkonium chloride (neat)	63449-41-2 (another possible CAS # is 8001-54-5, which is reported in NICEATM ALTTOX)	Ammonium salt| Benzyl	S	Y	NICEATM	Sigma-Aldrich	≥95%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	Possibly CO pers D21 (at least)	at least 1/3	**CO = 4**	1/3	Study terminated on D14 with CO = 3 in 1/3, CO = 2 in 2/3, IR = 1 in 3/3, CR = 1 in 2/3, CR = 0 in 1/3 and CC = 2 in 3/3; CO = 4 between D1 and D2 in 1/3	X
146	beta-Resorcylic acid	89-86-1	Carboxylic acid| Phenol	S	Y	ZEBET	Sigma-Aldrich	≥97%	1 of 1	Cat 1	CO mean ≥ 3	1/1	Unknown		**CO = 4**	1/1	Study terminated on D3 with CO = 4 in 1/1; CO = 4 between D1 and D3	X

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
147	Chlorhexidine	55-56-1	Aryl halide| Guanidine	S	Y	ECETOC / ZEBET	Sigma-Aldrich	≥99.5%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	Unknown		**CO = 4**	1/3	Study terminated on D3 with CO = 4 in 1/3, CO = 3 in 1/3 and CO = 2 in 1/3; CO = 4 between Hr1 and D3 in 1/3; Two studies are reported in ECETOC and ZEBET with the exact same animal scores (apart from 1 single CO score for animal 2 on D3, probably a typo) and are considered duplicate entries	X
148	Chlorophenacyl	6305-04-0	Alkyl halide| Ketone| Phenol	S	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	Cat 1	NA		Unknown		**CO = 4**	4/6	10 mg dose; Study terminated on D3 with CO = 4 in 3/6, CO = 3 in 2/6 and CO = 2 in 1/6; CO = 4 between D1 and D2 in 1/6, between D2 and D3 in 2/6 and on D3 in 1/6	
149	Granuform (Chemical name: Paraformaldehyde)	30525-89-4	Alcohol	S	Y	ZEBET	Sigma-Aldrich	95%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; at least 2/3	Unknown		**CO = 4**	1/3	Study terminated on D3 with CO = 4 in 1/1; CO = 4 on D3	X
150	N-(2-Methylphenyl)-iminodicarbonimidic diamide (1-(o-Tolyl)biguanide)	93-69-6	Aryl| Guanidine	S	Y	ZEBET	Sigma-Aldrich	98%	1 of 1	Cat 1	NA		Unknown		**CO = 4**	3/3	Study terminated after Hr1; Considered Cat 1 based on consistency of CO = 4 in 3/3	
151	N-Acetyl-DL-methionine	1115-47-5	Carboxamide| Sarcosine| Sulfide	S	Y	ZEBET	Sigma-Aldrich	99%	1 of 1	Cat 1	CO mean ≥ 1	3/3	Unknown		**CO = 4**	1/3	Study terminated on D3 with CO = 4 in 1/3; CO = 4 between Hr1 and D3	X
152	Sodium disilicate	13870-28-5	N/A	S	Y	ZEBET	Unknown	Unknown	1 of 1	Cat 1	NA		Unknown		**CO = 4**	3/3	Study terminated on D1 with CO = 4 in 3/3; CO = 4 on D1 in 3/3	?
153	Sodium hydrogen sulphate	7681-38-1	N/A	S	Y	ZEBET	Sigma-Aldrich	95%	1 of 1	Cat 1	NA		Unknown		**CO = 4**	1/1	Study terminated on D2 with CO = 4 in 1/1; CO = 4 between D1 and D2	X
154	Sodium silicate (2.0 ratio hydrous)	1344-09-8	N/A	S	Y	NICEATM	PQ Corporation; Samarth Chemical Products	Unknown	1 of 1	Cat 1	NA		Unknown		**CO = 4**	1/6	Study terminated on D3; No data reported for D1 to D3 in 3/6, for D1 to D2 in 1/6 and for D2 to D3 in 1/6 (obscured); CO = 4 on D1 in 1/6; CO = 0 on D3 in 2/6; 10 mg dose	X
155	Thiourea	62-56-6	Thiourea derivatives	S	Y	LNS / ECETOC	Sigma-Aldrich	≥99%	1 of 1	Cat 1	Conj mean ≥ 2; CO mean ≥ 1; IR mean ≥ 1	3/3; 2/3; 2/3			**CO = 4**	2/3	In LNS: CO = 4 on Hr1 in 2/3 fully reversed by D7 and D21 respectively. Animal 1 with full reversibility of all endpoints on D14 (CO on D7, max CO = 4), animal 2 on D14 (CO on D2, max CO = 2) and animal 3 on D21 (CO on D21, max CO = 4); In ECETOC 2/3 died (no mor	X
156	Triethanolamine orthovanadate (neat)	13476-99-8	Diketone	S	Y	NICEATM	Sigma-Aldrich	97%	1 of 1	Cat 1	NA		Unknown		**CO = 4**	4/6	Delayed effects; Study terminated on D7 with CO = 4 in 4/6, CO = 2 in 1/6 and CO = 0 in 1/6; CO & IR data missing for D1; CO = 4 on D7 in 3/6 and between D2 and D7 in 1/6	
157	2-(N-Methyl-2-pyridylamino)ethanol	122321-04-4	Alcohol| Aryl| Pyridine	L	Y	EURL ECVAM	Chemos GmbH	99%	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	1/1; 1/1; 1/1	Unknown		**Other observations**	1/1	Study terminated on D20; Pannus formation	X
158	1-(3,4-Dichlorophenyl)-5-isopropylbiguanide HCL	537-21-3	Aryl halide| Guanidine| Isopropyl	S	N	NICEATM	Toronto Research Chemicals	Unknown	1 of 1	Cat 1	NA		Unknown		**Other observations**	1/1	Study terminated on D1; Translucent corneal opacity, iridal inflammation, severe conjunctivitis with dulling of normal lustre of cornea, hemorrhage of iris, pale appearance of nictitating and lower conjunctival membranes; Animal sacrificed due to severity of reaction	X
159	2-Nitro-4-thiocyanoaniline	54029-45-7	Aniline| Nitrobenzene| Thiocyanate	S	Y	NICEATM	Sigma-Aldrich	95%	1 of 1	Cat 1	NA		Unknown		**Other observations**	1/1	Orange staining of cornea; Study terminated on D1	(X)
160	4-[(4-Amino-3-methylphenyl)(4-imino-3-methyl-2,5-cyclohexadien-1-ylidene)methyl]-2-methyl benzenamine hydrochloride	3248-91-7	Alkyl| Anilines| Benzyl| Conjugated hydrocarbon| Dianilines| Ketimine	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	Cat 1	NA		Unknown		**Other observations**	1/1	Colour staining of cornea; Study terminated on D1	(X)
161	Iodine chloride with pyridine (1:1)	6443-90-9	Aryl| Pyridine	S	Y	NICEATM	Unknown	Unknown	1 of 1	Cat 1	NA		Unknown		**Other observations**	1/1	Study terminated after Hr1; Dulling of cornea; Animal sacrificed due to severity of reaction	X
162	Phosphoric acid compound with 4-[(2,6-dichlorophenyl)(4-imino-3,5-dimethyl-2,5-cyclohexadien-1-ylidene)methyl]-2,6-dimethylaniline (1:1) (neat)	74578-10-2	Alkene| Alkyl| Aryl| Aryl halide| Ketimine| Precursors quinoid compounds	S	Y	Cosmetics Europe	Proprietary	≥95%	1 of 1	Cat 1	NA		Unknown		**Other observations**	1/1	Blue staining of cornea; Study terminated on D10	(X)/?
163	Tetra-N-octylammonium bromide	14866-33-2	Ammonium salt	S	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	Cat 1	NA		Unknown		**Other observations**	1/1	Study terminated after Hr6; Translucent corneal opacity, iridal inflammation and severe conjunctivitis with petechial hemorrhage scattered over nictitating membrane and blood stained discharge; Animal sacrificed due to severity of reaction	X
164	Iso-Propyl dicyanamide	35695-36-4	Cyanamide| Isopropyl	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	Cat 1	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	1/1; 1/1; 1/1	Unknown		**Other observations**	1/1	Study terminated on D3; Translucent corneal opacity, iridal inflammation, severe conjunctivitis with dulling of normal lustre of cornea, hemorrhage and pale appearance of nictitating membrane; Animal sacrificed due to severity of reaction	X
165	Mebrophen hydramide HCL	13977-28-1	Aliphatic Amine, tertiary| Aryl| Aryl halide| Ether	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	Cat 1	NA		Unknown		**Other observations**	1/1	Study terminated on D1; Grade 3 opacity over 1/2 with grade 2 over remaining half; Pale appearance of lower conjunctival membrane and white area on nictitating membrane; Areas of hemorrhage scattered over nictitating membrane; Opalescent corneal opacity, iridal inflammation, and severe conjunctivitis, pale appearance of lower conjunctival membrane and white area and hemorrhage over nictitating membrane; Abnormally small pupil; Animal sacrificed due to severe ocular reactions and pain and discomfort	X
166	2,6-Dichlorobenzoyl chloride	4659-45-4	Acyl halide| Aryl halide	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	6/6; 6/6	**Conj pers D7**; CO pers D7	6/6; 2/6				
167	2-Ethyl-1-hexanol	104-76-7	Alcohol| Alkane, branched with tertiary carbon	L	Y	ECETOC	Sigma-Aldrich	≥99.6%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	4/4; 3/4	**Conj pers D7**; CO pers D7	3/4; 1/4				
168	Acetone	67-64-1	Ketone	L	Y	ECETOC	Sigma-Aldrich	≥99.9%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	4/4; 4/4; 4/4	**Conj pers D7**; CO pers D7; IR pers D7	4/4; 1/4; 1/4				
169	Chlorhexidine gluconate (20%, aqueous)	18472-51-0	Aryl halide| Carboxylic acid| Dihydroxyl group| Guanidine	L	Y	NICEATM	Sigma-Aldrich	20%, aqueous	1 of 1	Cat 2A	**CO mean ≥ 1**	3/3	**CO pers D7**	1/3				
170	Cyclopentanol	96-41-3	Alcohol| Cycloalkane	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	3/3; 3/3	**CO pers D7**; Conj pers D7	1/3; 1/3				
171	Ethanol (neat) (2 of 4)	64-17-5	Alcohol	L	Y	ECETOC	Sigma-Aldrich	>99.8%	2 of 4	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	2/3; 2/3	**Conj pers D7**	2/3				X
172	Ethyl trans-3-ethoxyacrylate	5941-55-9	Acrylate| Alkoxy| Ether	L	Y	EURL ECVAM	Alfa Aesar	98%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3	**Conj pers D7**; IR pers D7; CO pers D7	3/3; 2/3; 1/3				
173	gamma-Butyrolactone (1 of 2)	96-48-0	Lactone| Oxolane| Saturated heterocyclic fragment	L	Y	ECETOC	TCI	>99%	1 of 2	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	3/3; 3/3	**Conj pers D7**; CO pers D7	2/3; 1/3				
174	gamma-Butyrolactone (2 of 2)	96-48-0	Lactone| Oxolane| Saturated heterocyclic fragment	L	Y	LNS	TCI	>99%	2 of 2	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 2/3; 2/3	**Conj pers D7**; CO pers D7	2/3; 1/3				
175	Iso-Butanol (1 of 2)	78-83-1	Alcohol| Isopropyl	L	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 2	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	4/4; 4/4	**Conj pers D7**; CO pers D7	4/4; 1/4				X
176	Methyl acetate (1 of 2)	79-20-9	Acetoxy| Carboxylic acid ester	L	Y	ECETOC	Sigma-Aldrich	≥99.8%	1 of 2	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	3/4; 3/4	**Conj pers D7**; CO pers D7	4/4; 1/4				(X)
177	Methyl ethyl ketone	78-93-3	Ketone	L	Y	ECETOC	Sigma-Aldrich	≥99.7%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	3/4; 3/4	**Conj pers D7**	3/4				
178	Methyl N,N,N-trimethyl-4-[(4,7,7-trimethyl-3-oxobicyclo[2.2.1]hept-2-ylidene)methyl]anilinium sulphate (30%, aqueous) (1 of 2)	52793-97-2	Alkene| Aromatic amine| Bicycloheptane| Bridged-ring carbocycles| Cycloalkane| Cycloketone| Sulfate	L	Y	EURL ECVAM	Proprietary	30%, aqueous	1 of 2	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**Conj pers D7**	3/3				?
179	n-Butanol (neat) (2 of 2)	71-36-3	Alcohol	L	Y	ECETOC	Sigma-Aldrich	99.8%	2 of 2	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	4/4; 4/4	**Conj pers D7**; CO pers D7	3/4; 1/4				X
180	n-Hexanol	111-27-3	Alcohol	L	Y	ECETOC	Sigma-Aldrich	≥99.5%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	4/4; 4/4	**Conj pers D7**	4/4				
181	n-Octanol (1 of 2)	111-87-5	Alcohol	L	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 2	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 2/3; 2/3	**Conj pers D7**; CO pers D7	2/3; 1/3				(X)
182	Polyether E810 (Chemical name: Polyether polyol)	25214-63-5	N/A	L	Y	NICEATM	Bayer	95-100%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	3/3; 3/3	**Conj pers D7**	3/3				
183	Propasol Solvent P	1569-01-3	Alcohol| Alkoxy| Ether	L	Y	NICEATM	Sigma-Aldrich	99%	1 of 1	Cat 2A	**CO mean ≥ 1**	5/6	**CO pers D7**; Conj pers D7	1/6; 1/6				
184	Pyridine (2 of 2)	110-86-1	Aryl| Pyridine	L	Y	LNS	Sigma-Aldrich	>99.9%	2 of 2	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3	**Conj pers D7**; CO pers D7	3/3; 2/3				X
185	Cetyl pyridinium bromide (1%)	140-72-7	Ammonium salt| Aryl| Pyridine	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 4/6	**Conj pers D7**; CO pers D7; IR pers D7	6/6; 3/6; 2/6				
186	Deoxycholic acid Na salt (10%)	302-95-4	Alkane, branched with tertiary carbon| Carboxylic acid| Cycloalkane| Dihydroxyl group	L (tested in solvent, available as S)	Y	LNS	Sigma-Aldrich	≥98%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**Conj pers D7**; CO pers D7	2/3; 1/3				
187	Lauryl sulphobetaine (10%)	14933-08-5	Ammonium salt| Sulfonic acid	L (tested in solvent, available as S)	Y	LNS	Sigma-Aldrich	≥97%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	3/3; 3/3	**Conj pers D7**; CO pers D7	3/3; 2/3				
188	Sodium lauryl sulphate (30%)	151-21-3	Alkoxy| Sulfate	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 4/6	**Conj pers D7**; CO pers D7	3/6; 1/6				X
189	Sodium lauryl sulphate (10%) (3 of 3)	151-21-3	Alkoxy| Sulfate	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99%	3 of 3	Cat 2A	**CO mean ≥ 1**	2/3	**CO pers D7**; Conj pers D7	1/3; 1/3				X
190	(2R,3R)-3-[(R)-1-(Tert-butyldimethylsiloxy)ethyl]-4-oxoazetidin-2-yl acetate	76855-69-1	Acetoxy| AlkoxySilane| Lactam| tert-Butyl	S	Y	EURL ECVAM	Chemos GmbH	99.8%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**CO pers D7**; Conj pers D7	3/3; 3/3				
191	3,3'-Dithiopropionic acid	1119-62-6	Carboxylic acid| Disulfide	S	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	Cat 2A	**CO mean ≥ 1**	3/3	**CO pers D7**	1/3				
192	4-Carboxybenzaldehyde	619-66-9	Aldehyde| Aryl| Carboxylic acid	S	Y	ECETOC	Sigma-Aldrich	97%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**CO pers D7**; Conj pers D7	2/3; 2/3				

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											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
193	6,7-Dihydro-2,3-dimethyl-imidazo[1,2-a]pyridin-8(5H)-one	362525-73-3	Aryl| Cycloketone| Fused saturated heterocycles| Fused unsaturated heterocycles| Imidazole| Piperidine| Saturated heterocyclic amine| Saturated heterocyclic fragment	S	Y	EURL ECVAM	Proprietary	>99.8%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3	**Conj pers D7**; IR pers D7	3/3; 1/3				?
194	Dibenzyl phosphate	1623-08-1	Benzyl| Phosphate ester	S	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	3/3; 3/3	**Conj pers D7**; CO pers D7	3/3; 1/3				
195	Disodium (E)-1,2-bis-(4-{4-methylamino-6-[4-methylcarbamoylphenylamino]-1,3,5-triazin-2-ylamino}phenyl-2-sulphonato)ethene	1808850-95-7	Alkene| Arene| Carboxamide| Melamines| Sulfonic acid	S	Y	EURL ECVAM	Proprietary	Unknown	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	5/6; 4/6	**CO pers D7**; Conj pers D7; IR pers D7	3/6; 3/6; 2/6				?
196	gamma-(Aminocarbonyl)-N-methyl-N,N-bis(1-methylethyl)-gamma-phenyl-, iodide	71-81-8	Ammonium salt| Aryl| Carboxamide| Isopropyl	S	Y	NICEATM	SCBT	Unknown	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**CO pers D7**; Conj pers D7	1/3; 1/3				
197	Methyl (2E)-[2-(chloromethyl)phenyl](methoxyimino) acetate	189813-45-4	Alkyl halide| Benzyl| Carboxylic acid ester| Ketoxime derivatives	S	Y	EURL ECVAM	Proprietary	100%	1 of 1	Cat 2A	**CO mean ≥ 1**; Conj mean ≥ 2	3/3; 3/3	**Conj pers D7**	3/3				?
198	Tetra aminopyrimidine sulphate (1 of 2)	5392-28-9	Anilines| Anilines(meta)| Anilines(ortho)| Anilines(para)	S	Y	LNS	Sigma-Aldrich	97%	1 of 2	Cat 2A	**CO mean ≥ 1**	2/3	**CO pers D7**; Conj pers D7	1/3; 1/3				X
199	Alkyl (C10-16) glucoside sodium carboxylate (~30%, aqueous)	383178-66-3	Dihydroxyl group	L	Y	EURL ECVAM	Proprietary	~30%, aqueous	1 of 1	Cat 2A	**Conj mean ≥ 2**; IR mean ≥ 1	3/3; 2/3	**Conj pers D7**	1/3				?
200	Allyl alcohol	107-18-6	Alcohol| Allyl	L	Y	LNS	Sigma-Aldrich	≥99%	1 of 1	Cat 2A	**Conj mean ≥ 2**; CO mean ≥ 1; IR mean ≥ 1	3/3; 2/3; 2/3	**Conj pers D7**	3/3				
201	Ethanol (neat) (3 of 4)	64-17-5	Alcohol	L	Y	LNS	Sigma-Aldrich	>99.8%	3 of 4	Cat 2A	**Conj mean ≥ 2**	2/3	**CO pers D7**; Conj pers D7	1/3; 1/3				X
202	Furfural	98-01-1	Alpha,beta unsaturated aldehyde| Aryl| Furane	L	Y	EURL ECVAM	Sigma-Aldrich	99%	1 of 1	Cat 2A	**Conj mean ≥ 2**	2/3	**Conj pers D7**; CO pers D7	3/3; 1/3				
203	Iso-Propanol	67-63-0	Alcohol| Isopropyl	L	Y	ECETOC	Sigma-Aldrich	≥99.7%	1 of 1	Cat 2A	**Conj mean ≥ 2**	3/4	**Conj pers D7**	4/4				
204	Methyl cyanoacetate	105-34-0	Carboxylic acid ester| Nitrile	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	Cat 2A	**Conj mean ≥ 2**; IR mean ≥ 1	3/3; 3/3	**Conj pers D7**	2/3				
205	Methyl N,N,N-trimethyl-4-[(4,7,7-trimethyl-3-oxobicyclo[2.2.1]hept-2-ylidene)methyl]anilinium sulphate (30%, aqueous) (2 of 2)	52793-97-2	Alkene| Aromatic amine| Bicycloheptane| Bridged-ring carbocycles| Cycloalkane| Cycloketone| Sulfate	L	Y	EURL ECVAM	Proprietary	30%, aqueous	2 of 2	Cat 2A	**Conj mean ≥ 2**	2/3	**Conj pers D7**	3/3				?
206	o-Toluene diamine, propoxylated, ethoxylated	67800-94-6	Epoxide| Precursors quinoid compounds| Saturated heterocyclic fraement	L	Y	NICEATM	Dow	100%	1 of 1	Cat 2A	**Conj mean ≥ 2**	3/3	**Conj pers D7**	2/3				
207	Triton X-100 (5%) (1 of 2)	9002-93-1	Alcohol| Alkane branched with quaternary carbon| Aryl| Ether| tert-Butyl	L	Y	ECETOC	Sigma-Aldrich	laboratory grade	1 of 2	Cat 2A	**Conj mean ≥ 2**; CO mean ≥ 1	6/6; 4/6	**Conj pers D7**	2/6				
208	Igepon AC-78 (5%) (Chemical name: Sodium cocoyl isethionate)	58969-27-0 (original CAS # deleted and replaced by 61789-32-0)	Carboxylic acid ester| Sulfonic acid	L (tested in solvent, neat chemical unknown)	Y	ECETOC	Unknown	Unknown	1 of 1	Cat 2A	**Conj mean ≥ 2**; CO mean ≥ 1	6/6; 5/6	**Conj pers D7**	6/6				?
209	N-Lauroyl sarcosine Na salt (10%)	137-16-6 (7631-98-3 reported by Gautheron et al. 1994, which corresponds to N-Dodecyl sarcosine Na salt or Sodium lauryl sarcosine)	Carboxamide| Carboxylic acid	L (tested in solvent, available as S)	Y	LNS	Sigma-Aldrich	≥99%	1 of 1	Cat 2A	**Conj mean ≥ 2**; CO mean ≥ 1	3/3; 2/3	**Conj pers D7**	1/3			Gautheron et al. 1994 reports CAS # 7631-98-3; However, it also mentions that the chemical tested was supplied by Sigma with catalogue number L5125, which in fact corresponds to CAS # 137-16-6	X
210	Sodium hydroxide (1%)	1310-73-2	Hydrazine	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	≥98%	1 of 1	Cat 2A	**Conj mean ≥ 2**	3/4	**Conj pers D7**	1/4				
211	1,3-bis-(2,4-Diaminophenoxy) propane tetrachloride	74918-21-1	Aminoaniline, meta| Ether	S	Y	EURL ECVAM	Chemos GmbH	99.3%	1 of 1	Cat 2A	**Conj mean ≥ 2**	3/3	**Conj pers D7**	2/3				
212	1,5-Naphthalenediol	83-56-7	Fused carbocyclic aromatic| Naphtalene| Phenol	S	Y	EURL ECVAM	Sigma-Aldrich	97%	1 of 1	Cat 2A	**Conj mean ≥ 2**	3/3	**Conj pers D7**	3/3				
213	2-Amino-3-hydroxy pyridine	16867-03-1	Heterocyclic Phenol	S	Y	EURL ECVAM	Sigma-Aldrich	98%	1 of 1	Cat 2A	**Conj mean ≥ 2**	3/3	**Conj pers D7**	3/3				
214	4-Amino-3-nitrophenol	610-81-1	Anilines| Nitro| Phenol	S	Y	EURL ECVAM	Sigma-Aldrich	98%	1 of 1	Cat 2A	**Conj mean ≥ 2**; CO mean ≥ 1	3/3; 2/3	**Conj pers D7**	1/3				
215	Ammonium nitrate	6484-52-2	Inorganic Salt	S	Y	ECETOC	Sigma-Aldrich	≥99.5%	1 of 1	Cat 2A	**Conj mean ≥ 2**	3/3	**Conj pers D7**	1/3				
216	Sodium benzoate	532-32-1	Aryl| Carboxylic acid	S	Y	EURL ECVAM	Sigma-Aldrich	≥99%	1 of 1	Cat 2A	**Conj mean ≥ 2**	3/3	**Conj pers D7**	3/3				
217	Butoxyethanol (3 of 3)	111-76-2	Alcohol| Alkoxy| Ether	L	Y	EURL ECVAM	Sigma-Aldrich	≥99%	3 of 3	Cat 2	**Conj mean ≥ 2**; CO mean ≥ 1	3/3; 2/3	Unknown				No scoring recorded on D7: unable to distinguish between Cat 2A and Cat 2B	X
218	2-Methyl-1-pentanol	105-30-6	Alcohol| Alkane, branched with tertiary carbon	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	Cat 2B	**CO mean ≥ 1**	2/3						
219	3-Chloropropionitrile	542-76-7	Alkyl halide| Nitrile	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	Cat 2B	**CO mean ≥ 1**	2/3						
220	Alcohol SDA 39C (79%)	64-17-5 (Ethanol) 84-66-6 (Diethylphthalate)	Ethanol	L	Y	NICEATM	Fisher Scientific; PHARMCO-AAPER	Unknown	1 of 1	Cat 2B	**CO mean ≥ 1**; Conj mean ≥ 2	3/3; 3/3					SDA = special denatured alcohol (99.01% (v/v) Ethanol + 0.99% (v/v) Diethylphthalate)	X
221	Butyl Dipropasol Solvent	29911-27-1	Alcohol| Alkoxy| Ether	L	Y	NICEATM	Sigma-Aldrich	≥98.5%	1 of 1	Cat 2B	**CO mean ≥ 1**	4/6						
222	Diethyl toluamide	134-62-3	Benzamide	L	Y	EURL ECVAM	Chemos GmbH	98%	1 of 1	Cat 2B	**CO mean ≥ 1**	3/3						
223	Ethyl-2-methyl acetoacetate	609-14-3	Carboxylic acid ester| Ketone	L	Y	ECETOC	Sigma-Aldrich	90%	1 of 1	Cat 2B	**CO mean ≥ 1**	2/3						
224	Iso-Butanal	78-84-2	Aldehyde| Isopropyl	L	Y	ZEBET	Sigma-Aldrich	≥99.5%	1 of 1	Cat 2B	**CO mean ≥ 1**; Conj mean ≥ 2	2/3; 2/3						
225	Methyl acetate (2 of 2)	79-20-9	Acetoxy| Carboxylic acid ester	L	Y	ZEBET	Sigma-Aldrich	≥99.8%	2 of 2	Cat 2B	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3						(X)
226	Monoethanolamine (10%)	141-43-5	Alcohol| Aliphatic Amine, primary	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	Cat 2B	**CO mean ≥ 1**	2/3						
227	n-Butanal	123-72-8	Aldehyde	L	Y	ZEBET	Sigma-Aldrich	≥99.5%	1 of 1	Cat 2B	**CO mean ≥ 1**; Conj mean ≥ 2	2/3; 2/3						
228	n-Octanol (2 of 2)	111-87-5	Alcohol	L	Y	LNS	Sigma-Aldrich	≥99%	2 of 2	Cat 2B	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	2/3; 2/3; 2/3						(X)
229	2,6-Dichloro-5-fluoro-beta-oxo-3-pyridinepropanoate	96568-04-6	Aromatic heterocyclic halide| Aryl halide| Carboxylic acid ester| Ketone	S	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	Cat 2B	**CO mean ≥ 1**	2/3						
230	2-Methyl-1,1'-biphenyl-3-ylmethyl (Z)-3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl cyclopropane carboxylate	82657-04-3	Alkenyl halide| Biphenyl| Carboxylic acid ester| Cycloalkane| Perhalogenated carbons derivatives	S	Y	EURL ECVAM	Chemos GmbH	97.1%	1 of 1	Cat 2B	**CO mean ≥ 1**	4/6						
231	2-Methyl-2-butanone-(4-sulfonamidophenyl) hydrazone	Unknown	N/A	S	Y	NICEATM	Unknown	Unknown	1 of 1	Cat 2B	**CO mean ≥ 1**; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3					Scores not recorded for D7; D8 scores show full reversibility for all endpoints; Assumed to be Cat 2B	?
232	Acetoacetic acid glycol ester	5459-04-1	Carboxylic acid ester| Diketone	S	N	ZEBET	Unknown	Unknown	1 of 1	Cat 2B	**CO mean ≥ 1**; Conj mean ≥ 2	2/3; 2/3						?
233	2-Pseudoionone	141-10-6	Alkene| Allyl| Conjugated system| Ketone	L	Y	ZEBET	Sigma-Aldrich	≥90%	1 of 1	Cat 2B	**Conj mean ≥ 2**	2/3						
234	Iso-Propyl acetoacetate	542-08-5	Carboxylic acid ester| Isopropyl| Ketone	L	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 1	Cat 2B	**Conj mean ≥ 2**	2/3						
235	Lupranol 3402 (Chemical name: Ethylenediamine, propoxylated)	25214-63-5	N/A	L	Y	NICEATM	BASF	100%	1 of 1	Cat 2B	**Conj mean ≥ 2**; CO mean ≥ 1	3/3; 2/3						
236	S-Bioallethrin	28434-00-6	Allyl| Carboxylic acid ester| Cycloalkane| Cycloalkene| Cycloketone	L	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	Cat 2B	**Conj mean ≥ 2**	5/6						

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
237	Glycolic acid (10%)	79-14-1	Alcohol| Carboxylic acid	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	99%	1 of 1	Cat 2B	**Conj mean ≥ 2**	2/3						
238	1,4-Dibutoxybenzene	104-36-9	Alkoxy| Aryl| Ether	S	Y	ZEBET	TCI	>98%	1 of 1	Cat 2B	**Conj mean ≥ 2**	3/3						
239	2-Hydroxy-1,4-naphthoquinone	83-72-7	Enol| Naphthoquinone	S	Y	EURL ECVAM	Sigma-Aldrich	97%	1 of 1	Cat 2B	**Conj mean ≥ 2**	2/3						
240	Camphene	79-92-5	Alkane, branched with tertiary carbon| Alkene| Bicycloheptane| Bridged-ring carbocycles| Cycloalkane	S	Y	ZEBET	Sigma-Aldrich	≥95%	1 of 1	Cat 2B	**Conj mean ≥ 2**	3/3						
241	m-Dinitrobenzene	99-65-0	Nitrobenzene	S	Y	ZEBET	Sigma-Aldrich	97%	1 of 1	Cat 2B	**Conj mean ≥ 2**; IR mean ≥ 1	2/3; 2/3						
242	p-Nitrobenzoic acid	62-23-7	Carboxylic acid| Nitrobenzene	S	Y	ZEBET	Sigma-Aldrich	≥98%	1 of 1	Cat 2B	**Conj mean ≥ 2**	3/3						
243	Sodium monochloroacetate	3926-62-3	Alkyl halide| Carboxylic acid	S	Y	ZEBET	Sigma-Aldrich	98%	1 of 1	Cat 2B	**Conj mean ≥ 2**	3/3						
244	Di-iso-propyl aminoethyldiphenyl acetamide	Unknown	N/A	S	N	NICEATM	Unknown	Unknown	1 of 1	Cat 2B	**IR mean ≥ 1**; CO mean ≥ 1; Conj mean ≥ 2	3/3; 2/3; 2/3						?
245	2,2-Dimethyl-3-pentanol	3970-62-5	Alcohol| Alkane branched with quaternary carbon| tert-Butyl	L	Y	ECETOC	Sigma-Aldrich	97%	1 of 1	No Cat	CO > 0 **	** CO 1/3						
246	2-Ethoxyethanol	110-80-5	Alcohol| Alkoxy| Ether	L	Y	LNS	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0 **	** CO 1/3						
247	3-Phenoxybenzyl alcohol	13826-35-2	Alcohol| Aryl| Benzyl| Ether	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO > 0 **	** CO 1/3						
248	alpha-Hexyl cinnamic aldehyde (12.5% in Acohol SDA 39C)	101-86-0	Alpha,beta unsaturated aldehyde| Benzyl	L	Y	NICEATM	Sigma-Aldrich (for alpha-Hexyl cinnamic aldehyde); Fisher Scientific (for Alcohol SDA 39C)	≥95%	1 of 1	No Cat	CO > 0 **	** CO 1/3; Conj 1/3						SDA = special denatured alcohol (99.01% (v/v) Ethanol + 0.99% (v/v) Diethylphthalate)	X
249	Benzotrichloride	98-07-7	Alkyl halide| Aryl	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO > 0 **	** Conj 3/6						
250	Cellosolve acetate	111-15-9	Acetoxy| Alkoxy| Carboxylic acid ester| Ether	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO > 0 **	** CO 1/4						
251	Cyclohexanone	108-94-1	Cycloalkane| Cycloketone	L	Y	LNS	Sigma-Aldrich	≥99.5%	1 of 1	No Cat	CO > 0 **	** CO 1/3						
252	Ethyl thioglycolate	623-51-8	Carboxylic acid ester| Thioalcohol	L	Y	ECETOC	Sigma-Aldrich	97%	1 of 1	No Cat	CO > 0 **	** CO 1/3; Conj 1/3; IR 1/3						
253	Ethyltrimethyl acetate	3938-95-2	Carboxylic acid ester| tert-Butyl	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO > 0 **	** CO 1/6						
254	Glycidyl methacrylate	106-91-2	Epoxide| Methacrylate| Saturated heterocyclic fragment	L	Y	ECETOC	Sigma-Aldrich	≥97%	1 of 1	No Cat	CO > 0 **	** CO 1/3; Conj 1/3; IR 1/3						
255	Lactic acid (10%)	50-21-5	Alcohol| Carboxylic acid	L	Y	NICEATM	Sigma-Aldrich	90%	1 of 1	No Cat	CO > 0 **	** Conj 1/3						
256	Methanol	67-56-1	Alcohol	L	Y	LNS	Sigma-Aldrich	≥99.9%	1 of 1	No Cat	CO > 0 **	** CO 1/3; Conj 1/3						
257	Methyl amyl ketone (1 of 2)	110-43-0	Ketone	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 2	No Cat	CO > 0 **	** Conj 1/4						
258	Methylal	109-87-5	Acetal	L	Y	NICEATM	Sigma-Aldrich	99%	1 of 1	No Cat	CO > 0 **	** CO 1/6					A second study is also reported in NICEATM ALTTOX with the exact same animal scores and is considered a duplicate entry	
259	Metolachlor	51218-45-2	Aryl| Ether| Haloacetamide	L	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO > 0 **	** Conj 1/6						
260	Phosphoric acid, tributyl ester (also known as Tributyl phosphate) (1 of 2)	126-73-8	Alkoxy| Phosphate ester	L	Y	NICEATM	Sigma-Aldrich	≥ 99%	1 of 2	No Cat	CO > 0 **	** CO 1/3; Conj 1/3						X
261	Polyalkenylsuccinate ester/amine salt	Unknown	N/A	L	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO > 0 **	** Conj 2/6						?
262	Trimethoxy(3,3,3-trifluoropropyl)silane	429-60-7	Alkoxy Silanes| Alkyl halide	L	Y	EURL ECVAM	Sigma-Aldrich	≥97%	1 of 1	No Cat	CO > 0 **	** Conj 1/3; IR 1/3						
263	Triton X-15 surfactant	9036-19-5	Alcohol| Alkane branched with quaternary carbon| Aryl| Ether| tert-Butyl	L	Y	NICEATM	Sigma-Aldrich	50-100%	1 of 1	No Cat	CO > 0 **	** CO 1/4; Conj 1/4						
264	Di-iso-propanolamine (10%)	110-97-4	Aliphatic Amine, secondary| Dihydroxyl group	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥ 98%	1 of 1	No Cat	CO > 0 **	** CO 1/3						
265	N-Lauroyl sarcosine Na salt (30%) (Sodium-N-lauroyl sarcosinate reported in NICEATM ALTTOX)	137-16-6	Carboxamide| Carboxylic acid	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0 **	** CO 1/3						X
266	Sodium lauryl sulphate (3%)	151-21-3	Alkoxy| Sulfate	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0 **	** CO 1/6						
267	1,2-Epoxycyclooctane	286-62-4	Cycloalkane| Epoxide| Fused saturated heterocycles| Saturated heterocyclic fragment	S	Y	ZEBET	Sigma-Aldrich	99%	1 of 1	No Cat	CO > 0 **	** CO 1/3						
268	Alcohol sulfate mono-C16-18	68955-20-4	Sulfate	S	Y	EURL ECVAM	Proprietary	93.4%	1 of 1	No Cat	CO > 0 **	** CO 2/4; Conj 2/4						?
269	Fluoxastrobin	361377-29-9	Aromatic heterocyclic halide| Aryl| Aryl halide| Ether| Ketoxime derivatives| Unsaturated heterocyclic fragment	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO > 0 **	** CO 1/3						
270	Iodosulphuron-methyl-sodium	144550-36-7	Aromatic heterocyclic halide| Aryl| Aryl halide| Carboxylic acid ester| Ether| Sulfonamide| Sulfonyl urea| Triazine| Urea derivatives	S	Y	EURL ECVAM	Chemos GmbH	90.8%	1 of 1	No Cat	CO > 0 **	** CO 1/3; Conj 1/3						
271	Sodium bisulphite	7631-90-5	Inorganic Salt	S	Y	ZEBET	Sigma-Aldrich	100%	1 of 1	No Cat	CO > 0 **	** CO 1/3; Conj 1/3						
272	2-Nitro-4-thio-N-propylaniline	54393-89-4	Aniline| Nitrobenzene| Sulfide	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO > 0 **	** Conj 1/3; IR 1/3						?
273	3-Hydroxy-2-phenyl-4-quinolinecarboxylic acid	485-89-2	Carboxylic acid| Heterocyclic Phenol| Quinoline/ isoquinoline	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO > 0 **	** CO 1/3; Conj 1/3; IR 1/3						?
274	p-tert-Butylbenzoic acid, triethanolamine salt (neat)	59993-86-1 (98-73-7 reported in NICEATM ALTTOX, which corresponds to 4-tert-Butylbenzoic acid)	Alcohol| Aliphatic Amine, tertiary| Aryl| Carboxylic acid| Isopropyl	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO > 0 **	** CO 1/6						?
275	1,2,3-Trichloropropane (1 of 2)	96-18-4	Alkyl halide	L	Y	LNS	Sigma-Aldrich	99%	1 of 2	No Cat	CO > 0							
276	2,4-Pentanedione	123-54-6	Diketone	L	Y	LNS	Sigma-Aldrich	≥99.5%	1 of 1	No Cat	CO > 0							
277	2-Ethylhexanoyl chloride (neat)	760-67-8	Acyl halide	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO > 0						CO = 2 on Hr1 in 1/6; CO = 1 on Hr1 in 1/6	
278	2-Methoxyethanol	109-86-4	Alcohol| Ether	L	Y	LNS	Sigma-Aldrich	≥99.9%	1 of 1	No Cat	CO > 0							
279	Dimethyl carbonate	616-38-6	Carbonate	L	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0							
280	Dimethyl sulfoxide (DMSO)	67-68-5	Sulfoxide	L	Y	LNS	Sigma-Aldrich	≥99.9%	1 of 1	No Cat	CO > 0						CO = 1 on Hr1 in 1/3	
281	Ethyl acetate	141-78-6	Acetoxy| Carboxylic acid ester	L	Y	ECETOC	Sigma-Aldrich	99.9%	1 of 1	No Cat	CO > 0							
282	Ethyl acetoacetate	141-97-9	Carboxylic acid ester| Ketone	L	Y	LNS	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0							
283	Furan	110-00-9	Aryl| Furane	L	Y	LNS	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0							
284	Methyl amyl ketone (2 of 2)	110-43-0	Ketone	L	Y	ECETOC	Sigma-Aldrich	99%	2 of 2	No Cat	CO > 0							

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
285	Methyl iso-butyl ketone (1 of 2)	108-10-1	Isopropyl| Ketone	L	Y	LNS	Sigma-Aldrich	≥99.5%	1 of 2	No Cat	CO > 0							
286	Methyl iso-butyl ketone (2 of 2)	108-10-1	Isopropyl| Ketone	L	Y	ECETOC	Sigma-Aldrich	≥99.5%	2 of 2	No Cat	CO > 0							
287	n-Butyl acetate	123-86-4	Acetoxy| Carboxylic acid ester	L	Y	ECETOC	Sigma-Aldrich	≥99.5%	1 of 1	No Cat	CO > 0							
288	Propiconazole	60207-90-1	Aryl| Aryl halide| Dioxolane| Saturated heterocyclic fragment| Triazole	L	Y	EURL ECVAM	Chemos GmbH	95.2%	1 of 1	No Cat	CO > 0							
289	Propylidynetrimethanol, propoxylated	25723-16-4	Alcohol| Alkane branched with quaternary carbon| Ether	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO > 0							
290	Sodium polyoxyethylene laurylether sulphate (27%, aqueous)	9004-82-4 (68585-34-2 reported in NICEATM ALTTOX, which corresponds to Sodium lauryl ether sulphate)	Alkoxy| Ether| Sulfate	L	Y	NICEATM	Oxiteno (ALKOPON® N)	27%, aqueous	1 of 1	No Cat	CO > 0							
291	Styrene	100-42-5	Alkene| Aryl	L	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0							
292	Triethanolamine (neat) (1 of 2)	102-71-6	Alcohol| Aliphatic Amine, tertiary	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 2	No Cat	CO > 0							
293	Triton X-155 (10%)	9010-44-0	N/A	L (tested in solvent, neat chemical unknown)	Y	LNS	Unknown	Unknown	1 of 1	No Cat	CO > 0						CO = 1 on Hr1 in 1/3	?
294	Cetyl pyridinium bromide (0.1%)	140-72-7	Ammonium salt| Aryl| Pyridine	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO > 0							
295	m-Phenylene diamine (10%)	108-45-2	Aminoaniline, meta	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0						CO = 1 between Hr1 and Hr4 in 1/3	
296	Sodium lauryl sulphate (1%) (1 of 2)	151-21-3	Alkoxy| Sulfate	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 2	No Cat	CO > 0						CO = 1 between Hr1 and Hr4 in 1/3	
297	Sodium lauryl sulphate (1%) (2 of 2)	151-21-3	Alkoxy| Sulfate	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99%	2 of 2	No Cat	CO > 0						CO = 1 on Hr4 in 1/3	
298	Sucrose fatty acid ester (10%)	Unknown	N/A	L (tested in solvent, available as S)	Y	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO > 0							?
299	(-)Phenylephrine	59-42-7	Alcohol| Aliphatic Amine, secondary| Phenol	S	Y	ZEBET	SCBT	98%	1 of 1	No Cat	CO > 0						CO = 1 on Hr1 in 1/4	
300	(+)Phenylephrine	614-03-9	Alcohol| Aliphatic Amine, secondary| Phenol	S	Y	ZEBET	Unknown	Unknown	1 of 1	No Cat	CO > 0							?
301	1,3,5-Trioxane	110-88-3	Acetal| Saturated heterocyclic fragment| Trioxane	S	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0						CO = 2 on Hr1 in 1/3	
302	1-Phenyl-3-pyrazolidone	92-43-3	Aryl| Pyrazolidinedione/ Pyrazolidone	S	Y	LNS	Sigma-Aldrich	97%	1 of 1	No Cat	CO > 0							
303	2,4-Dichloro-5-sulphamoyl-benzoic acid	2736-23-4	Aryl halide| Carboxylic acid| Sulfonamide	S	Y	LNS	Sigma-Aldrich	98%	1 of 1	No Cat	CO > 0							
304	2-(Acetyloxy)-1-phenylethanone	2243-35-8	Acetoxy| Aryl| Carboxylic acid ester| Ketone	S	Y	NICEATM	Alfa Aesar	98%	1 of 1	No Cat	CO > 0							
305	5-Chloro-3-methylbenzo[b]thiophene-2-sulphonyl chloride	166964-33-6	Alkyl| Aryl halide| Benzothiophene/ Benzoisothiophene| Sulfonyl halide	S	Y	NICEATM	Fisher Scientific	97%	1 of 1	No Cat	CO > 0							
306	5-Methyl-1,3,4-thiadiazol-2-amine	108-33-8	Amidine| Aryl| Thiadiazole	S	Y	ZEBET	Sigma-Aldrich	97%	1 of 1	No Cat	CO > 0						CO = 1 on Hr1 in 3/3	
307	6-Nitro-1,2,3,4-tetrahydroquinoxaline	41959-35-7	Fused saturated heterocycles| Nitrobenzene	S	Y	Cosmetics Europe	Fluorochem	≥95%	1 of 1	No Cat	CO > 0							
308	Acrylamidopropyltrimonium chloride/acrylamide copolymer	75150-29-7	Acrylamide| Ammonium salt	S	Y	EURL ECVAM	Proprietary	≥94%	1 of 1	No Cat	CO > 0							?
309	Betaine monohydrate	590-47-6	Ammonium salt| Carboxylic acid	S	Y	LNS	Sigma-Aldrich	99%	1 of 1	No Cat	CO > 0						CO = 1 on Hr1 in 2/3	
310	Bromethalin	63333-35-7	Alkyl halide| Aromatic amine| Aryl halide| Nitrobenzene	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO > 0							
311	Dimethyl biguanide	657-24-9	Guanidine	S	Y	LNS	Unknown	Unknown	1 of 1	No Cat	CO > 0							?
312	DL-Glutamic acid	19285-83-7	Alpha amino acid| Carboxylic acid	S	Y	LNS	Sigma-Aldrich	>99%	1 of 1	No Cat	CO > 0							
313	Ethylenediaminetetraacetic acid dipotassium salt (EDTA di-K salt)	25102-12-9	Aliphatic Amine, tertiary| Carboxylic acid	S	Y	LNS	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0							
314	Iminodibenzyl	494-19-9	Fused carbocyclic aromatic| Fused saturated heterocycles| Precursors quinoid compounds	S	Y	LNS	Sigma-Aldrich	97%	1 of 1	No Cat	CO > 0							
315	Magnesium carbonate	56378-72-4	N/A	S	Y	LNS	Sigma-Aldrich	99%	1 of 1	No Cat	CO > 0							
316	Propyl-4-hydroxybenzoate	94-13-3	Carboxylic acid ester| Phenol	S	Y	LNS	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO > 0							
317	Tetra aminopyrimidine sulphate (2 of 2)	5392-28-9	Anilines| Anilines(meta)| Anilines(ortho)| Anilines(para)	S	Y	ECETOC	Sigma-Aldrich	97%	2 of 2	No Cat	CO > 0							X
318	1-(5-Amino-2-methoxyphenyl) piperazine hydrochloride	Unknown (CAS # for 1-(5-Amino-2-methoxyphenyl) piperazine is 14856-46-90-1)	N/A	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO > 0							?
319	2-Nitro-4-propoxyaniline	20367-34-4	Alkoxy| Aniline| Ether| Nitrobenzene	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO > 0							?
320	Piperonyl butoxide	51-03-6	Alkoxy| Benzodioxole| Benzyl| Ether	L	Y	EURL ECVAM	Chemos GmbH	94.8%	1 of 1	No Cat	CO = 0 **	** Conj 2/6						
321	Toluene (1 of 2)	108-88-3	Aryl	L	Y	ECETOC	Sigma-Aldrich	≥99.9%	1 of 2	No Cat	CO = 0 **	** Conj 1/4						X
322	Xylene (1 of 2)	1330-20-7	Inside	L	Y	ECETOC	Sigma-Aldrich	≥98.5% (Xylene mixture of isomers)	1 of 2	No Cat	CO = 0 **	** Conj 1/4						
323	Triethanolamine orthovanadate (30%)	13476-99-8	Diketone	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	97%	1 of 1	No Cat	CO = 0 **	** Conj 2/6						
324	N,N-Dimethyl guanidine sulphate	598-65-2	Aliphatic Amine, tertiary| Amidine| Guanidine	S	Y	ECETOC	Sigma-Aldrich	97%	1 of 1	No Cat	CO = 0 **	** Conj 1/3						
325	6-(Methylamino)-2-pyridine ethanol formate (1:1) (salt)	Intermediate - No CAS	N/A	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0 **	** Conj 1/3						?
326	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate (9CI) and 1,2,3- Propanetricarboxylic acid, 2-hydroxy-, silver(1+) salt, monohydrate	Unknown	N/A	L	Y	EURL ECVAM	Proprietary	Unknown	1 of 1	No Cat	CO = 0							?
327	1,2,3-Trichloropropane (2 of 2)	96-18-4	Alkyl halide	L	Y	NICEATM	Sigma-Aldrich	99%	2 of 2	No Cat	CO = 0							
328	1,2,4-Trimethylbenzene	95-63-6	Aryl	L	Y	LNS	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
329	1,2,6-Hexanetriol	106-69-4	Alcohol| Dihydroxyl group	L	Y	ZEBET	Sigma-Aldrich	96%	1 of 1	No Cat	CO = 0							
330	1,3-Dibromopropane	109-64-8	Alkyl halide	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
331	1,3-Di-iso-propyl benzene	99-62-7	Aryl| Isopropyl	L	Y	ECETOC	Sigma-Aldrich	96%	1 of 1	No Cat	CO = 0							
332	1,4-Dibromobutane	110-52-1	Alkyl halide	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
333	1,5-Dibromopentane	111-24-0	Alkyl halide	L	Y	ECETOC	Sigma-Aldrich	97%	1 of 1	No Cat	CO = 0							
334	1,5-Hexadiene	592-42-7	Allyl	L	Y	ECETOC	Sigma-Aldrich	97%	1 of 1	No Cat	CO = 0							

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
335	1,6-Dibromohexane	629-03-8	Alkyl halide	L	Y	ECETOC	Sigma-Aldrich	96%	1 of 1	No Cat	CO = 0							
336	1,9-Decadiene	1647-16-1	Allyl	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
337	1-(2,6-Dimethylphenoxy)-2-propanol	61102-09-8 (53012-41-2 reported in ZEBET, which corresponds to 1-(2,6-Dimethylphenoxy)acetone)	Alcohol| Aryl| Ether	L	N	ZEBET	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
338	1-Bromo-4-chlorobutane	6940-78-9	Alkyl halide	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
339	1-Ethyl-3-methylimidazolium ethyl sulphate	342573-75-5	Alkoxy| Ammonium salt| Aryl| Imidazole| Sulfate	L	Y	EURL ECVAM	Sigma-Aldrich	≥95%	1 of 1	No Cat	CO = 0							
340	1-Methylpropylbenzene	135-98-8	Aryl	L	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
341	1-Nitropropane	108-03-2	Nitro aliphatic	L	Y	LNS	Sigma-Aldrich	≥98.5%	1 of 1	No Cat	CO = 0							
342	2,2',2"-Nitrilotriethanol, propoxylated	37208-53-0	Alcohol| Aliphatic Amine, tertiary| Ether	L	Y	NICEATM	Oltchim	>99%	1 of 1	No Cat	CO = 0							
343	2,4-Dicyano-1-butene	1572-52-7	Allyl| Nitrile	L	Y	NICEATM	TCI	>98%	1 of 1	No Cat	CO = 0							
344	2,4-Pentanediol	625-69-4	Dihydroxyl group	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
345	2-(2-Ethoxy-ethoxy) ethanol	111-90-0	Alcohol| Alkoxy| Ether	L	Y	EURL ECVAM	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
346	2-Chloro-2,4,4-trimethylpentane	6111-88-2	Alkane branched with quaternary carbon| Alkyl halide| tert-Butyl	L	Y	NICEATM	Fluorochem	100%	1 of 1	No Cat	CO = 0							
347	2-Ethoxyethyl methacrylate	2370-63-0	Alkoxy| Ether| Methacrylate	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
348	2-Ethylhexyl p-dimethylamino benzoate (10%)	21245-02-3	Alkane, branched with tertiary carbon| Aromatic amine| Carboxylic acid ester	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
349	2-Ethylhexyl p-dimethylamino benzoate (neat)	21245-02-3	Alkane, branched with tertiary carbon| Aromatic amine| Carboxylic acid ester	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
350	2-Ethylhexylthioglycolate	7659-86-1 (7659-86-12 reported in ECETOC, which is wrong)	Alkane, branched with tertiary carbon| Carboxylic acid ester| Thioalcohol	L	Y	ECETOC	Sigma-Aldrich	≥95%	1 of 1	No Cat	CO = 0							
351	2-Methoxy-3,4-dihydropyran (neat)	4454-05-1 (103-75-3 reported in NICEATM ALTTOX, which corresponds to 2-Ethoxy-3,4-dihydropyran)	Allyl| Dihydropyran| Ether| Unsaturated heterocyclic fragment	L	Y	NICEATM	TCI	>97%	1 of 1	No Cat	CO = 0							
352	2-Methylpentane	107-83-5	Isopropyl	L	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
353	2-Propylheptyl octanoate	868839-23-0	Alkane, branched with tertiary carbon| Carboxylic acid ester	L	Y	EURL ECVAM	Proprietary	Unknown	1 of 1	No Cat	CO = 0							?
354	3,3-Dimethylpentane	562-49-2	Alkane branched with quaternary carbon	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
355	3-Ethyl toluene	620-14-4	Aryl	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
356	3-Methoxy-1,2-propanediol	623-39-2	Dihydroxyl group| Ether| Glycerol and derivatives	L	Y	ECETOC	TCI	>98%	1 of 1	No Cat	CO = 0							
357	3-Methylhexane	589-34-4	Alkane, branched with tertiary carbon	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
358	3-Phenoxy benzaldehyde (neat) (1 of 2)	39515-51-0	Aldehyde| Aryl| Ether	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 2	No Cat	CO = 0							
359	3-Phenoxy benzaldehyde (neat) (2 of 2)	39515-51-0	Aldehyde| Aryl| Ether	L	Y	NICEATM	Sigma-Aldrich	98%	2 of 2	No Cat	CO = 0							
360	4-Bromophenetole	588-96-5 (589-10-6 reported in ECETOC, which corresponds to beta-Bromophenetole)	Alkoxy| Aryl halide| Ether	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
361	Allyl methacrylate	96-05-9	Allyl| Methacrylate	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
362	alpha-Hexyl cinnamic aldehyde (12.5% in Petrolatum (87.5%))	101-86-0	Alpha,beta unsaturated aldehyde| Benzyl	L	Y	NICEATM	Sigma-Aldrich (for alpha-Hexyl cinnamic aldehyde); Unknown (for Petrolatum)	≥95%	1 of 1	No Cat	CO = 0							X
363	alpha-Hexyl cinnamic aldehyde (6.25% in Alcohol SDA 39C)	101-86-0	Alpha,beta unsaturated aldehyde| Benzyl	L	Y	NICEATM	Sigma-Aldrich (for alpha-Hexyl cinnamic aldehyde); Fisher Scientific (for Alcohol SDA 39C)	≥95%	1 of 1	No Cat	CO = 0						SDA = special denatured alcohol (99.01% (v/v) Ethanol + 0.99% (v/v) Diethylphthalate)	X
364	Amyl acetate (neat)	628-63-7	Acetoxy| Carboxylic acid ester	L	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
365	Bicyclo [2,2,1]hept-5-ene-2-carbonitrile (P30671)	95-11-4	Bridged-ring carbocycles| Nitrile	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0						One of the six animals exhibited depression, emaciation and marked diarrhea; Death was noted prior to the 72 hour reading; From gross observation, death was not attributed to sample application	
366	Bisphenol A, diethylene triamine, epichlorohydrin polymer, ethoxylated, propoxylated (56%, aqueous emulsion)	455946-46-0	Alcohol| Aliphatic Amine, primary| Aliphatic Amine, secondary| Alkane, branched with quaternary carbon| Alkyl halide| Epoxide| Ether| Phenol| Saturated heterocyclic fragment	L	Y	EURL ECVAM	Proprietary	56%, aqueous	1 of 1	No Cat	CO = 0							?
367	Bisphenol A, epichlorohydrin polymer, ethoxylated, propoxylated (53-57%, aqueous emulsion)	68123-18-2	Alkyl halide| Epoxide| Phenol| Saturated heterocyclic fragment	L	Y	EURL ECVAM	Proprietary	~55%, aqueous	1 of 1	No Cat	CO = 0							?
368	bis-(3-Triethoxisilylpropyl)-tetrasulphide	40372-72-3	Alkoxy| AlkoxySilane| Sulfide, poly	L	Y	ZEBET	Sigma-Aldrich	≥90%	1 of 1	No Cat	CO = 0							
369	Bromo-2-butane	78-76-2	Alkyl halide	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
370	Carsonon N-9 (Chemical name: Nonyl phenol ethoxylate, branched) (neat)	9016-45-9 (127087-87-0 reported in NICEATM ALTTOX, which corresponds to Tergitol NI nonionic surfactants)	Alcohol| Benzyl| Ether	L	Y	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0						Data missing for D1	?
371	cis-Cyclooctene	931-87-3 (931-88-4 reported in ECETOC, which corresponds to Cyclooctene)	Allyl| Cycloalkene	L	Y	ECETOC	Sigma-Aldrich	95%	1 of 1	No Cat	CO = 0							
372	Clarified slurry oil	64741-62-4	Fused carbocyclic aromatic	L	Y	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
373	Dichlorotoluenes	Mixture	N/A	L	N	ECETOC	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
374	Dimethylhydropolysiloxane (neat)	68037-59-2	Allyl| Aryl halide| Benzamide| Sarcosine	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
375	Dimethyl siloxane, mono dimethylvinylsiloxy- and mono trimethoxysiloxy-terminated (95%)	471277-16-4	Alkene| AlkoxySilane| Silane	L	Y	EURL ECVAM	Proprietary	100%	1 of 1	No Cat	CO = 0							?
376	Dioctyl carbonate	1680-31-5	Carbonate	L	Y	EURL ECVAM	Proprietary	97%	1 of 1	No Cat	CO = 0							?
377	Dioctyl ether	629-82-3	Alkoxy| Ether	L	Y	EURL ECVAM	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
378	Di-iso-butyl ketone	108-83-8	Isopropyl| Ketone	L	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
379	Di-n-propyl disulphide	629-19-6	Disulfide	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
380	Dodecane	112-40-3	Methyl| Methylene	L	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							

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											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
381	Dow Corning Syltherm 444 heat transfer fluid (Chemical name: Polydimethylsiloxane)	63148-62-9	Silane	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
382	Dow Corning X201133 heat transfer fluid (Chemical name: Polydimethylsiloxane)	63148-62-9	Silane	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
383	Dynacylan VPS 8815 (Chemical name: Siloxanes and Silicones, 3-[[2-[[2-aminoethyl)amino]ethyl]amino]propyl hydroxy, hydroxy 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl, hydroxy-terminated, formates (salts))	273737-91-0	N/A	L	Y	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
384	Ethanol (10%)	64-17-5	Alcohol	L	Y	NICEATM	Sigma-Aldrich	>99.8%	1 of 1	No Cat	CO = 0							
385	Ethylene oxide	75-21-8	Epoxide| Saturated heterocyclic fragment	L	Y	NICEATM	Sigma-Aldrich	≥99.9%	1 of 1	No Cat	CO = 0						Liquefied gaz	
386	Ethyleneglycol diethyl ether	629-14-1	Alkoxy| Ether	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
387	Ethylthioethyl methacrylate	14216-25-2	Methacrylate| Sulfide	L	Y	ECETOC	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
388	Ethyltriglycol methacrylate	39670-09-2 (36670-09-2 reported in ECETOC, which is wrong)	Alkoxy| Ether| Methacrylate	L	Y	ECETOC	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
389	Fungitrol zinc 8% fungicide (Chemical name: Zinc naphthenate) (neat)	12001-85-3	Alkane, branched with tertiary carbon| Carboxylic acid| Cycloalkane	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
390	gamma-Chloropropyltrimethoxy silane (neat)	2530-87-2	AlkoxySilane| Alkyl halide	L	Y	NICEATM	Sigma-Aldrich	≥97%	1 of 1	No Cat	CO = 0							
391	gamma-Glycidyloxypropyltrimethoxy silane (3-Glycidoxypropyltrimethoxysilane reported in LNS) (1 of 2)	2530-83-8	AlkoxySilane| Epoxide| Ether| Saturated heterocyclic fragment	L	Y	LNS	Sigma-Aldrich	≥98%	1 of 2	No Cat	CO = 0							
392	gamma-Glycidyloxypropyltrimethoxy silane ((3-Glycidoxypropyl)trimethoxy silane reported in NICEATM ALTTOX) (2 of 2)	2530-83-8	AlkoxySilane| Epoxide| Ether| Saturated heterocyclic fragment	L	Y	NICEATM	Sigma-Aldrich	≥98%	2 of 2	No Cat	CO = 0							
393	gamma-Mercaptopropyl trimethoxy silane (3-Mercaptopropyl trimethoxy silane reported in NICEATM ALTTOX) (neat) (1 of 2)	4420-74-0 (2530-87-2 reported in NICEATM ALTTOX, which corresponds to 3-Chloropropyl trimethoxy silane)	AlkoxySilane| Thioalcohol	L	Y	NICEATM	Sigma-Aldrich	95%	1 of 2	No Cat	CO = 0							
394	gamma-Mercaptopropyl trimethoxy silane (neat) (2 of 2)	4420-74-0	AlkoxySilane| Thioalcohol	L	Y	NICEATM	Sigma-Aldrich	95%	2 of 2	No Cat	CO = 0							
395	gamma-Methacryloxypropyltrimethoxy silane	2530-85-0	AlkoxySilane| Methacrylate	L	Y	NICEATM	Sigma-Aldrich	≥98%	1 of 1	No Cat	CO = 0							
396	Genagen (Chemical name: Polyethylene glycol 400 dilaurate)	68139-91-3	Carboxylic acid ester| Ether	L	N	ZEBET	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
397	Genomoll P (Chemical name: Tris(2-chloroethyl) phosphate)	115-96-8	Alkyl halide| Phosphate ester	L	Y	ZEBET	Sigma-Aldrich	97%	1 of 1	No Cat	CO = 0							
398	Glycadiol	556-52-5	Alcohol| Epoxide| Saturated heterocyclic fragment	L	Y	ZEBET	Sigma-Aldrich	96%	1 of 1	No Cat	CO = 0							
399	Glycerol (Glycerin reported in NICEATM ALTTOX) (10%)	56-81-5	Dihydroxyl group| Glycerol and derivatives	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	No Cat	CO = 0							
400	Glycerol (Glycerin reported in NICEATM ALTTOX) (neat) (1 of 2)	56-81-5	Dihydroxyl group| Glycerol and derivatives	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 2	No Cat	CO = 0							
401	Glycerol (neat) (2 of 2)	56-81-5	Dihydroxyl group| Glycerol and derivatives	L	Y	ECETOC	Sigma-Aldrich	≥99.5%	2 of 2	No Cat	CO = 0							
402	Glycerol tri-iso-stearate	26492-95-5	N/A	L	N	ECETOC	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
403	Heptyl methacrylate	5459-37-0	Methacrylate	L	Y	ECETOC	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
404	Hexahydrofarnesylacetone	502-69-2	Alkane, branched with tertiary carbon| Isopropyl| Ketone	L	Y	ZEBET	Bedoukian Research, Inc.	98%	1 of 1	No Cat	CO = 0							
405	Igepal CO-210 (Chemical name: Nonyl phenol ethoxylate, branched)	68412-54-4 or 9016-45-9 or 26027-38-3 (84852-15-3 reported in NICEATM ALTOX, which is wrong)	Alcohol| Benzyl| Ether	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							X
406	Igepal CO-990 (Chemical name: Nonyl phenol ethoxylate, branched)	68412-54-4 or 9016-45-9 or 26027-38-3 (84852-15-3 reported in NICEATM ALTOX, which is wrong)	Alcohol| Benzyl| Ether	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							X
407	Iron pentacarbonyl (neat)	13463-40-6	N/A	L	Y	NICEATM	Sigma-Aldrich	≥99.99%	1 of 1	No Cat	CO = 0							
408	iso-Bornyl acetate	125-12-2	Acetoxy| Alkane, branched with tertiary carbon| Bicycloheptane| Bridged-ring carbocycles| Carboxylic acid ester| Cycloalkane	L	Y	ZEBET	Sigma-Aldrich	≥95%	1 of 1	No Cat	CO = 0							
409	iso-Nonylaldehyde	5435-64-3 (35127-50-5 reported in ZEBET, which corresponds to Isononan-1-al)	Aldehyde| Alkane branched with quaternary carbon| Alkane, branched with tertiary carbon| tert-Butyl	L	Y	ZEBET	Sigma-Aldrich	≥95%	1 of 1	No Cat	CO = 0							
410	iso-Octyl acrylate	29590-42-9	Acrylate| Isopropyl	L	Y	ECETOC	Sigma-Aldrich	>90%	1 of 1	No Cat	CO = 0							
411	iso-Octyl thioglycolate	25103-09-7	Carboxylic acid ester| Isopropyl| Thioalcohol	L	Y	ECETOC	Merck	≥98%	1 of 1	No Cat	CO = 0							
412	iso-Propyl bromide	75-26-3	Alkyl halide| Isopropyl	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
413	iso-Propyl iso-stearate	68171-33-5	Carboxylic acid ester| Isopropyl	L	N	ECETOC	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
414	iso-Propyl myristate (10%)	110-27-0	Carboxylic acid ester| Isopropyl	L	Y	NICEATM	Sigma-Aldrich	≥98%	1 of 1	No Cat	CO = 0							
415	iso-Propyl myristate (neat)	110-27-0	Carboxylic acid ester| Isopropyl	L	Y	NICEATM	Sigma-Aldrich	≥98%	1 of 1	No Cat	CO = 0							
416	iso-Stearic acid	30399-84-9	Carboxylic acid| Isopropyl	L	Y	ECETOC	Jarchem	Unknown	1 of 1	No Cat	CO = 0							
417	iso-Stearyl alcohol	27458-93-1	Alcohol| Isopropyl	L	Y	ECETOC	Jarchem	100%	1 of 1	No Cat	CO = 0							
418	Kerosine	8008-20-6	N/A	L	Y	NICEATM	Sigma-Aldrich	100%	1 of 1	No Cat	CO = 0							
419	Kronitex 100 (Chemical name: synthetic iso-Propylphenyl phosohate)	Unknown (possibly 66797-44-2)	N/A	L	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
420	Kronitex 200 (Chemical name: synthetic iso-Propylphenyl phosphate)	Unknown (possibly 96300-97-9)	N/A	L	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
421	Kronitex 200B (Chemical name: tert-Butylphenyl phosphate)	Unknown	N/A	L	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
422	Kronitex 300 (Chemical name: iso-Propylphenyl phosphate)	Unknown (possibly 67426-58-8)	N/A	L	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
423	Kronitex 50 (Chemical name: synthetic iso-Propylphenyl phosphate)	Unknown (possibly 67426-57-7)	N/A	L	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
424	Kronitex CDP (Chemical name: Cresyl diphenyl phosphate)	26444-49-5	Aryl| Phosphate ester	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
425	Kronitex TXP (Chemical name: Trixylenyl phosphate) (1 of 2)	68952-33-0	Benzyl| Phosphate ester	L	N	NICEATM	Unknown	Unknown	1 of 2	No Cat	CO = 0							?
426	Kronitex TXP (Chemical name: Trixylenyl phosphate) (2 of 2)	68952-33-0	Benzyl| Phosphate ester	L	N	NICEATM	Unknown	Unknown	2 of 2	No Cat	CO = 0							?
427	Methyl cyclopentadiene dimer	26472-00-4	Alkane, branched with tertiary carbon| Alkyl| Cycloalkene	L	Y	NICEATM	Sigma-Aldrich	93%	1 of 1	No Cat	CO = 0							
428	Methyl cyclopentane	96-37-7	Alkane, branched with tertiary carbon| Cycloalkane	L	Y	ECETOC	Sigma-Aldrich	97%	1 of 1	No Cat	CO = 0							
429	Methyl triglycol	112-35-6	Alcohol| Ether	L	Y	ZEBET	Sigma-Aldrich	≥97%	1 of 1	No Cat	CO = 0							
430	Methyl trimethyl acetate	598-98-1	Carboxylic acid ester| tert-Butyl	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
431	Methyl tetraglycol	23783-42-8 (9004-74-4 reported in ZEBET, which corresponds to Poly(ethylene glycol) methyl ether)	Alcohol| Ether	L	Y	ZEBET	TCI	≥98%	1 of 1	No Cat	CO = 0							
432	m-Methoxthybenzaldehyde	591-31-1	Aldehyde| Aryl| Ether	L	Y	ZEBET	Sigma-Aldrich	≥97%	1 of 1	No Cat	CO = 0							
433	Nitrobenzene	98-95-3	Nitrobenzene	L	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							

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											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
434	Nonyl acrylate	2664-55-3	Acrylate	L	Y	ECETOC	Monomer-Polymer and Dajac Labs	Unknown	1 of 1	No Cat	CO = 0							
435	Nonyl methacrylate	13453-03-7	Alkane branched with quaternary carbon| Alkane, branched with tertiary carbon| Methacrylate| tert-Butyl	L	Y	ECETOC	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
436	n-Amyl bromide	110-53-2	Alkyl halide	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
437	n-Hexane	110-54-3	N/A	L	Y	LNS	Sigma-Aldrich	≥97%	1 of 1	No Cat	CO = 0							
438	n-Hexyl bromide	111-25-1	Alkyl halide	L	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
439	Octadecyl isocyanate	112-96-9	Isocyanate	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
440	Organofunctional silane S3-98 (neat)	26115-70-8	N/A	L	Y	NICEATM	SCBT	>98%	1 of 1	No Cat	CO = 0							
441	n-Octyl bromide	111-83-1	Alkyl halide	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
442	Pentaerythritol, propoxylated	9051-49-4	Alcohol| Alkane branched with quaternary carbon| Dihydroxyl group| Ether	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
443	Perfluoro-n-hexane (1 of 2)	355-42-0	Perfluorocarbons derivatives	L	Y	NICEATM	Sigma-Aldrich	99%	1 of 2	No Cat	CO = 0							
444	Perfluoro-n-hexane (2 of 2)	355-42-0	Perfluorocarbons derivatives	L	Y	NICEATM	Sigma-Aldrich	99%	2 of 2	No Cat	CO = 0							
445	Petroleum ether	8032-32-4	N/A	L	Y	LNS	Sigma-Aldrich	100%	1 of 1	No Cat	CO = 0							
446	Phosphoric acid, tributyl ester (Tributyl phosphate reported in NICEATM ALTTOXI (2 of 2)	126-73-8	Alkoxy| Phosphate ester	L	Y	NICEATM	Sigma-Aldrich	≥99%	2 of 2	No Cat	CO = 0							X
447	Polyethylene glycol 400 (10%)	25322-68-3	Dihydroxyl group	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
448	Polyethylene glycol 400 (neat) (1 of 2)	25322-68-3	Dihydroxyl group	L	Y	ECETOC	Sigma-Aldrich	Unknown	1 of 2	No Cat	CO = 0							
449	Polyethylene glycol 400 (neat) (2 of 2)	25322-68-3	Dihydroxyl group	L	Y	NICEATM	Sigma-Aldrich	Unknown	2 of 2	No Cat	CO = 0							
450	Polyethylene glycol 600	25322-68-3	Dihydroxyl group	L	Y	ECETOC	Fisher Scientific	>95%	1 of 1	No Cat	CO = 0							
451	Polyethylene glycol dimethylether	24991-55-7	Ether	L	Y	ZEBET	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
452	Polyethylene glycol monolaurate	9004-81-3	Alcohol| Carboxylic acid ester	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
453	Polyglyceryl-3-diisooctadecanoate	63705-03-3	Alcohol| Carboxylic acid ester| Isopropyl	L	Y	EURL ECVAM	Proprietary	100%	1 of 1	No Cat	CO = 0							?
454	Polyol 355 UCB	25791-96-2	Alcohol| Ether| Glycerol and derivatives	L	Y	NICEATM	Dow	>99%	1 of 1	No Cat	CO = 0							
455	Polyol XZ 95435.00	52625-13-5	Alcohol| Dihydroxyl group| Ether	L	Y	NICEATM	Dow	>99%	1 of 1	No Cat	CO = 0							
456	Propylene glycol	57-55-6	Dihydroxyl group	L	Y	ECETOC	Sigma-Aldrich	≥99.5%	1 of 1	No Cat	CO = 0							
457	p-Chlorobenzotrifluoride	98-56-6	Alkyl halide| Aryl halide	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
458	p-Methyl thiobenzaldehyde	3446-89-7	Aldehyde| Aryl| Sulfide	L	Y	ECETOC	Sigma-Aldrich	95%	1 of 1	No Cat	CO = 0							
459	p-tert-Butylbenzoic acid, triethanolamine salt (10%)	59993-86-1 (98-73-7 reported in NICEATM ALTTOX, which corresponds to 4-tert-Butylbenzoic acid)	Alcohol| Aliphatic Amine, tertiary| Aryl| Carboxylic acid| Isopropyl	L	Y	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
460	Ricinoleic acid tin salt	71828-07-4	Dihydroxyl group	L	Y	EURL ECVAM	Proprietary	100%	1 of 1	No Cat	CO = 0							?
461	Silan 108 (Chemical name: Trimethoxyoctylsilane)	3069-40-7	AlkoxySilane	L	Y	ZEBET	Sigma-Aldrich	96%	1 of 1	No Cat	CO = 0							
462	Silicone Y-4081 (Chemical name: Hexamethyldisiloxane) (neat)	107-46-0	Disiloxane	L	Y	NICEATM	Sigma-Aldrich	≥98.5%	1 of 1	No Cat	CO = 0							
463	Steareth-10 allyl ether/acrylates copolymer (~40%, aqueous)	109292-17-3	Acrylate| Alkoxy| Allyl| Carboxylic acid| Ether	L	Y	EURL ECVAM	Proprietary	~40%, aqueous	1 of 1	No Cat	CO = 0							?
464	Thiodiglycol	111-48-8	Alcohol| Sulfide	L	Y	ECETOC	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
465	Tricresyl phosphate (Kronitex TCP reported in NICEATM ALTTOXI (1 of 2)	1330-78-5	Aryl| Phosphate ester	L	Y	NICEATM	Sigma-Aldrich	90%	1 of 2	No Cat	CO = 0							
466	Tricresyl phosphate (2 of 2)	1330-78-5	Aryl| Phosphate ester	L	Y	NICEATM	Sigma-Aldrich	90%	2 of 2	No Cat	CO = 0							
467	Triethanolamine (10%)	102-71-6	Alcohol| Aliphatic Amine, tertiary	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	No Cat	CO = 0							
468	Triethanolamine (neat) (2 of 2)	102-71-6	Alcohol| Aliphatic Amine, tertiary	L	Y	LNS	Sigma-Aldrich	≥99.5%	2 of 2	No Cat	CO = 0							
469	Triethoxyoctylsilane (neat)	2943-75-1	Alkoxy| AlkoxySilane	L	Y	NICEATM	Sigma-Aldrich	≥97.5%	1 of 1	No Cat	CO = 0							
470	Triethylene glycol	112-27-6	Alcohol| Ether	L	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
471	Trifluoroethyl methacrylate	352-87-4 (392-68-7 reported in ECETOC, which corresponds to Ethyl trifluoroacrylate)	Allyl halide| Methacrylate	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
472	Trisodecyl phosphite (neat)	25448-25-3	N/A	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
473	Trisoctylamine	25549-16-0	Aliphatic Amine, tertiary| Isopropyl	L	Y	ZEBET	Merck	≥95%	1 of 1	No Cat	CO = 0							
474	Triphenyl phosphite (neat)	101-02-0	Aryl| Phosphite ester	L	Y	NICEATM	Sigma-Aldrich	97%	1 of 1	No Cat	CO = 0							
475	Triton X-100 (1%)	9002-93-1	Alcohol| Alkane branched with quaternary carbon| Aryl| Ether| tert-Butyl	L	Y	ECETOC	Sigma-Aldrich	laboratory grade	1 of 1	No Cat	CO = 0							
476	Tween 20 (1 of 2)	9005-64-5	Acetal| Alcohol| Allyl| Carboxylic acid ester| Ether| Oxolane| Saturated heterocyclic fragment	L	Y	ECETOC	Sigma-Aldrich	Unknown	1 of 2	No Cat	CO = 0							
477	Tween 20 (2 of 2)	9005-64-5	Acetal| Alcohol| Allyl| Carboxylic acid ester| Ether| Oxolane| Saturated heterocyclic fragement	L	Y	NICEATM	Sigma-Aldrich	Unknown	2 of 2	No Cat	CO = 0							
478	Tween 80 (10%)	9005-65-6	Acetal| Alcohol| Allyl| Carboxylic acid ester| Ether| Oxolane| Saturated heterocyclic fragment	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
479	Tween 80 (neat)	9005-65-6	Acetal| Alcohol| Allyl| Carboxylic acid ester| Ether| Oxolane| Saturated heterocyclic fragment	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
480	Vinyl 2-ethylhexanoate (neat)	94-04-2	Alkene| Carboxylic acid ester	L	Y	NICEATM	TCI	>98%	1 of 1	No Cat	CO = 0							
481	Vinyl tris (beta-methoxyethoxy) silane	1067-53-4	N/A	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
482	Vinyltrimethoxy silane	2768-02-7	N/A	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							

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											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
483	Xylene (2 of 2)	1330-20-7	Ittide	L	Y	ECETOC	Sigma-Aldrich	≥98.5% (Xylene mixture of isomers)	2 of 2	No Cat	CO = 0							
484	Igepon AC-78 (0.5%) (Chemical name: Sodium cocoyl isethionate)	58969-27-0 (original CAS # deleted and replaced by 61789-32-0)	Carboxylic acid ester| Sulfonic acid	L (tested in solvent, neat chemical unknown)	Y	ECETOC	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
485	Acid Red 92 (Chemical name: 3,4,5,6-Tetrachloro-2-(1,4,5,8-tetrabromo-6-hydroxy-3-oxoxanthen-9-yl)-benzoic acid) (1%)	18472-87-2	Aromatic perhalogencarbons| Aryl halide| Fused carbocyclic aromatic| Fused saturated heterocycles| Heterocyclic spiro rings| Isobenzofuran| Lactone| Phenol| Xanthene	L (tested in solvent, available as S)	Y	NICEATM	SCBT	>95%	1 of 1	No Cat	CO = 0							
486	Benzyl alcohol (1%)	100-51-6	Alcohol| Benzyl	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	99.80%	1 of 1	No Cat	CO = 0							
487	Brij-35 (10%) (Chemical name: Polyoxyethylene 23 lauryl ether; also known as Brij L23)	9002-92-0	Alcohol| Alkoxy| Ether	L (tested in solvent, available as S)	Y	LNS	Sigma-Aldrich	100%	1 of 1	No Cat	CO = 0							
488	Calcium thioglycolate (10%)	814-77-1	N/A	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥98%	1 of 1	No Cat	CO = 0							
489	Cetylpyridinium chloride (0.1%)	6004-24-6	Ammonium salt| Aryl| Pyridine	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	>99%	1 of 1	No Cat	CO = 0							
490	Ivory soap solution (5%, aqueous)	Unknown	N/A	L (tested in solvent, available as S)	Y	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
491	Myrj-45 (10%) (Chemical name: Polyoxyethylene 8-stearate)	9004-99-3	Alcohol| Carboxylic acid ester	L (tested in solvent, available as S)	Y	LNS	Croda	Unknown	1 of 1	No Cat	CO = 0							
492	Phosphoric acid compound with 4-[(2,6-dichlorophenyl)(4-imino-3,5-dimethyl-2,5-cyclohexadien-1-ylidene)methyl]-2,6-dimethylaniline (1:1) (2% (w/v), aqueous)	74578-10-2	Alkene| Allyl| Aryl| Aryl halide| Ketimine| Precursors quinoid compounds	L (tested in solvent, available as S)	Y	Cosmetics Europe	Proprietary	≥95%	1 of 1	No Cat	CO = 0							?
493	Sodium chloride isotonic solution	7647-14-5	N/A	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	No Cat	CO = 0							
494	Sodium salicylate (10%)	54-21-7	Carboxylic acid| Phenol	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	No Cat	CO = 0							
495	Theophylline sodium (0.1%)	3485-82-3	Dihydropurinedione| Urea derivatives	L (tested in solvent, available as S)	Y	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0						NICEATM ALTTOX database indicates 0.1 in the concentration field; Not clear if this is percent concentration or dose volume inserted by mistake in the concentration field	?
496	Trichloroacetic acid (3%)	76-03-9	Alkyl halide| Carboxylic acid	L (tested in solvent, available as S)	Y	ECETOC	Sigma-Aldrich	>99%	1 of 1	No Cat	CO = 0							
497	Triethanolamine orthovanadate (3%)	13476-99-8	Diketone	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	97%	1 of 1	No Cat	CO = 0							
498	2-(7-Ethyl-1H-indol-3-yl)-ethanol	41340-36-7	Alcohol| Allyl| Benzyl| Indole/ Isoindole	S (waxy)	Y	EURL ECVAM	Chemos GmbH	99.2%	1 of 1	No Cat	CO = 0							
499	Perfecto petrolatum	Unknown	N/A	S (waxy)	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
500	Polyethylene glycol (PEG-120) methyl glucose dioleate	86893-19-8	Acetal| Alcohol| Allyl| Carboxylic acid ester| Ether| Ether (cyclic)| Heterocyclic fragment	S (waxy)	Y	EURL ECVAM	Proprietary	100%	1 of 1	No Cat	CO = 0							?
501	Polyethylene glycol (PEG-40) hydrogenated castor oil (Polyoxyethylene hydrogenated castor oil reported in NICEATM ALTTOX) (1 of 2)	61788-85-0	Acylal| Alcohol| Allyl| Ether	S (waxy)	Y	NICEATM	Sigma-Aldrich	100%	1 of 2	No Cat	CO = 0							
502	Polyethylene glycol (PEG-40) hydrogenated castor oil (2 of 2)	61788-85-0	Acylal| Alcohol| Allyl| Ether	S (waxy)	Y	EURL ECVAM	Sigma-Aldrich	100%	2 of 2	No Cat	CO = 0							
503	[3-Chloro-4-[[3-fluorobenzyl]oxy]phenyl][6-iodoquinazolin-4-yl]amine	231278-20-9	Aromatic amine| Aryl| Aryl halide| Benzyl| Ether| Quinazoline	S	Y	EURL ECVAM	Chemos GmbH	99%	1 of 1	No Cat	CO = 0							
504	1,5-Di(2,4-dimethylphenyl)-3-methyl-1,3,5-triazapenta-1,4-diene	33089-61-1	Amidine| Aryl	S	Y	EURL ECVAM	Chemos GmbH	98.1%	1 of 1	No Cat	CO = 0							
505	1,6,7,12-Tetrachloro-3,4,9,10-tetracarbonic acid anhydride	156028-26-1	N/A	S	Y	ZEBET	SCBT	98%	1 of 1	No Cat	CO = 0							
506	1H-Indole-2,3-dione	91-56-5	Cycloketone| Indoline| Lactams	S	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
507	1-(4-Chlorophenyl)-3-(3,4-dichlorophenyl) urea	101-20-2	Aromatic heterocyclic halide| Aryl halide| Urea derivatives	S	Y	EURL ECVAM	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
508	1-(4-Phenyl-phenoxy)-1-(1,2,4-triazole-1)-3,3-dimethylbutan-2-ol	55179-31-2	Alcohol| Alkane, branched with quaternary carbon| Biphenyl| Ether| Hydrazone	S	Y	NICEATM	SCBT	100%	1 of 1	No Cat	CO = 0							
509	1-(9H-Carbazol-4-yloxy)-3-[[2-(2-methoxyphenoxy)ethyl]amino]propan-2-ol	72956-09-3	Alcohol| Aliphatic Amine, secondary| Aryl| Carbazole| Ether	S	Y	EURL ECVAM	Chemos GmbH	99.8%	1 of 1	No Cat	CO = 0							
510	2',6',8-Trifluoro-5-methoxy[1,2,4]triazolo[1,5-c]pyrimidine-2-sulphonanilide	145701-23-1	Amidine| Aromatic heterocyclic halide| Aryl halide| Ether| Sulfonamide	S	Y	EURL ECVAM	Chemos GmbH	98.9%	1 of 1	No Cat	CO = 0							
511	2,2'-[[3-Methyl-4-[(4-nitrophenyl)azo]phenyl]imino]bis-ethanol	3179-89-3	Alcohol| Aromatic amine| Aryl| Azo| Nitrobenzene	S	Y	EURL ECVAM	Chemos GmbH	100%	1 of 1	No Cat	CO = 0							
512	2,2'-[[4-[(2-Methoxyethyl)amino]-3-nitrophenyl]imino]bis-ethanol	23920-15-2	Alcohol| Aromatic amine| Ether| Nitrobenzene	S	Y	EURL ECVAM	Chemos GmbH	99.3%	1 of 1	No Cat	CO = 0							
513	2,2'-[6-(4-Methoxyphenyl)-1,3,5-triazine-2,4-diyl]bis[5-[(2-ethylhexyl)oxy]-phenol]	187393-00-6	Alkoxy| Aryl| Ether| Phenol| Triazine	S	Y	EURL ECVAM	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
514	2,2'-Methylene-bis-(6-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol)	103597-45-1	Alkane branched with quaternary carbon| Aryl| Benzyl| Fused carbocyclic aromatic| Fused saturated heterocycles| Phenol| tert-Butyl	S	Y	EURL ECVAM	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
515	2,3-Dimethyl-2,3-dinitrobutane	3964-18-9 (3964-18-4 reported in NICEATM ALTTOX, which is wrong)	Nitro-aliphatic	S	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
516	2,5,6-Triamino-4-pyrimidinol sulphate	1603-02-7	Aryl| Pyrimidine| Sulfate	S	Y	EURL ECVAM	ChemReagents.com	94%	1 of 1	No Cat	CO = 0							
517	2,6-Dihydroxy-3,4-dimethylpyridine	84540-47-6	Heterocyclic Phenol	S	Y	EURL ECVAM	Chemos GmbH	98.5%	1 of 1	No Cat	CO = 0							

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											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
518	2-(4-Oxopentyl)-1H-isoindole-1,3 (2H)-dione	3197-25-9	Aryl| Fused carbocyclic aromatic| Fused saturated heterocycles| Imide| Ketone	S	Y	NICEATM	SCBT	≥95%	1 of 1	No Cat	CO = 0							
519	2-(Diphenylacetyl)-1,3-indandione	82-66-6	Aryl| Diketone| Indandione	S	Y	EURL ECVAM	Chemos GmbH	95.2%	1 of 1	No Cat	CO = 0							
520	2-(n-Dodecylthio)ethanol	1462-55-1	Alcohol| Sulfide	S	Y	ECETOC	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
521	2-Aminophenol	95-55-6	Precursors quinoid compounds	S	Y	LNS	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
522	2-Anilino-4,6-dimethylpyrimidine	53112-28-0	Aromatic amine| Aryl| Pyrimidine	S	Y	EURL ECVAM	Chemos GmbH	98.2%	1 of 1	No Cat	CO = 0							
523	2-Hydroxyethyliminodisodium acetate	135-37-5	Alcohol| Aliphatic Amine, tertiary| Carboxylic acid	S	Y	ZEBET	American Custom Chemicals Corporation	>95%	1 of 1	No Cat	CO = 0							
524	2-Mercaptopyrimidine	1450-85-7	Heterocyclic Thiophenol	S	Y	LNS	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
525	3,4-Dimethoxybenzaldehyde	120-14-9	Aldehyde| Aryl| Ether	S	Y	NICEATM	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
526	3,5-Dihydroxyacetophenone	51863-60-6 (35086-59-0 reported in ZEBET, which corresponds to 3',5'-Diacetoxyacetophenone)	Ketone| Phenol	S	Y	ZEBET	Sigma-Aldrich	97%	1 of 1	No Cat	CO = 0							
527	3H-Pyrazole-3-one, 2(4-aminophenyl),4-dihydro-5-(1-pyrrolidinyl)	30707-77-8	Amidine| Aniline| Pyrazolone| Pyrrolidine| Saturated heterocyclic amine| Saturated heterocyclic fragment	S	Y	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
528	3-((Benzylthio)methyl)-6-chloro-1,1-dioxide	91-33-8	Aryl| Aryl halide| Benzyl| Sulfide| Sulfonamide| Unsaturated heterocyclic fragment	S	Y	NICEATM	SCBT	>98%	1 of 1	No Cat	CO = 0							
529	3-(2-Chloro-thiazol-5-ylmethyl)-5-methyl[1,3,5]oxadiazinan-4-ylidene-N-nitroamine	153719-23-4	Allyl| Aryl halide| Guanidine| Saturated heterocyclic fragment	S	Y	EURL ECVAM	Chemos GmbH	96.3%	1 of 1	No Cat	CO = 0							
530	3-Chloro-4-fluoronitrobenzene	350-30-1 (446-35-5 reported in ECETOC, which corresponds to 2,4-Difluoronitrobenzene)	Aryl halide| Nitrobenzene	S	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
531	4'-Aminoazobenzene-4-sulphonic acid	104-23-4	Aniline| Aryl| Azo| Sulfonic acid	S	Y	ZEBET	IS Chemical Technology	98%	1 of 1	No Cat	CO = 0							
532	4,4'-Methylene bis-(2,6-di-tert-butylphenol)	118-82-1 (118-82-3 reported in ECETOC, which is wrong)	Benzyl| Phenol| tert-Butyl	S	Y	ECETOC	Sigma-Aldrich	98%	1 of 1	No Cat	CO = 0							
533	4,4'-Sulfonylbisbenzenamide	80-08-0	Dianilines| Sulfone	S	Y	NICEATM	Sigma-Aldrich	97%	1 of 1	No Cat	CO = 0							
534	4,4-Dimethyl-3-oxopentanitrile	59997-51-2	Ketone| Nitrile| tert-Butyl	S	Y	ZEBET	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
535	4-Chloro-4-nitrodiphenylether	1836-74-4	Aryl| Aryl halide| Ether| Nitrobenzene	S	Y	ZEBET	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
536	Abamectin	71751-41-2	Acetal| Alkane, branched with tertiary carbon| Allyl| Cycloalkene| Dihydroxyl group| Ether| Ether, cyclic| Heterocyclic spiro rings| Lactone| Saturated heterocyclic fragment| Unsaturated heterocyclic fragment	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO = 0							
537	Aluminium hydroxide	21645-51-2	N/A	S	Y	LNS	Sigma-Aldrich	reagent grade	1 of 1	No Cat	CO = 0							
538	Ambuphylline	5634-34-4	Alcohol| Aliphatic Amine, primary| Dihydropurinedione| Urea derivatives	S	Y	ZEBET	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
539	Amicarbazone	129909-90-6	Amidine| Carboxamide| Hydrazine| Hydrazone| Imide| Lactam	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO = 0							
540	Anthracene	120-12-7	Anthracene| Fused carbocyclic aromatic	S	Y	LNS	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
541	Benzoflex S-312 (Chemical name: Neopentyl glycol dibenzoate)	4196-89-8	Alkane branched with quaternary carbon| Aryl| Carboxylic acid ester	S	Y	NICEATM	TCI	>98%	1 of 1	No Cat	CO = 0							
542	beta-(4-Chlorophenoxy)-alpha-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol	55219-65-3	Alcohol| Alkane branched with quaternary carbon| Aryl| Aryl halide| Ether| tert-Butyl| Triazole	S	Y	NICEATM	SCBT	≥96%	1 of 1	No Cat	CO = 0							
543	Brodifacoum	56073-10-0	Aryl| Aryl halide| Biphenyl| Chromene| Enol| Fused carbocyclic aromatic| Lactone| Tetralin	S	Y	NICEATM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO = 0							
544	Caffeine sodium benzoate	8000-95-1	N/A	S	Y	ZEBET	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
545	Caffeine sodium salicylate	8002-85-5	N/A	S	Y	ZEBET	Carbone Scientific	98%	1 of 1	No Cat	CO = 0							
546	Cellulose,2-(2-hydroxy-3-(trimethylammonium)propoxy)ethyl ether chloride(91%)	68610-92-4	Alcohol| Ammonium salt| Ether	S	Y	EURL ECVAM	Sigma-Aldrich	91%	1 of 1	No Cat	CO = 0							
547	Chlorpyrifos	2921-88-2	Alkoxy| Aromatic heterocyclic halide| Aryl halide| Thiophosphate	S	Y	NICEATM	SCBT	≥98%	1 of 1	No Cat	CO = 0							
548	Dequest 2016	29329-71-3	Alcohol| Phosphonic acid	S	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0						No CAS # reported in NICEATM ALTTOX; CAS No. 29329-71-3 (x-Na), 3794-83-0 (4-Na), depends on the # of Na ions	?
549	Disperse red 60 (Chemical name: 1-amino-4-hydroxy-2-phenoxy-9,10-anthracenedione)	17418-58-5	Aniline| Anthracenone/ Antracendione| Aryl| Ether| Phenol	S	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	No Cat	CO = 0							
550	EPIKURE 1061	2716-10-1	N/A	S	Y	NICEATM	Sigma-Aldrich	99%	1 of 1	No Cat	CO = 0							
551	EPIKURE 1062	2716-12-3	N/A	S	Y	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
552	EPIKOTE RSS 1079	47758-37-2	Aryl| Ether| Fluorene| Saturated heterocyclic fragment	S	Y	NICEATM	TCI	>98%	1 of 1	No Cat	CO = 0							

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
553	Etoxazole	153233-91-1	Alkoxy| Aryl| Aryl halide| Ether| tert-Butyl| Unsaturated heterocyclic fragment	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO = 0							
554	Famoxadone	131807-57-3	Aryl| Carbamate| Ether| Imide| Oxazolidine derivatives| Saturated heterocyclic fragment	S	Y	EURL ECVAM	Toronto Research Chemicals	Unknown	1 of 1	No Cat	CO = 0							
555	Fenamidone	161326-34-7	Aryl| Imidazoline| Sulfide| Unsaturated heterocyclic amine| Unsaturated heterocyclic fragment	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO = 0							
556	Flonicamid	158062-67-0	Alkyl halide| Aryl| Carboxamide| Nitrile| Pyridine	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO = 0							
557	Fluopicolide	239110-15-7	Alkyl halide| Aromatic heterocyclic halide| Aryl halide| Benzamide	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO = 0							
558	Gluconolactone	90-80-2	Dihydroxyl group| Lactone| Saturated heterocyclic fragment	S	Y	LNS	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
559	Hexabromocyclododecane	25637-99-4	Alkyl halide| Cycloalkane	S	Y	NICEATM	MPI Chemie BV	≥98%	1 of 1	No Cat	CO = 0							
560	Hexamethylenetetraamine	100-97-0	Bridged-ring heterocycles| Saturated heterocyclic amine| Saturated heterocyclic fragment	S	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
561	Hexyl 2-(1-(diethylaminohydroxyphenyl)methanoyl) benzoate	302776-68-7	Aromatic amine| Aryl| Carboxylic acid ester| Ketone| Phenol	S	Y	EURL ECVAM	Sigma-Aldrich	≥98%	1 of 1	No Cat	CO = 0							
562	Methyl p-hydroxybenzoate (neat)	99-76-3	Carboxylic acid ester| Phenol	S	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
563	Myristyl myristate	3234-85-3	Carboxylic acid ester	S	Y	ECETOC	Chemos GmbH	98.4%	1 of 1	No Cat	CO = 0							
564	N-Allyl-N-(4-amino-2-nitrophenyl)amine	160219-76-1	Allyl| Aniline| Nitrobenzene	S	Y	Cosmetics Europe	Proprietary	>98%	1 of 1	No Cat	CO = 0							?
565	Phenothiazine	92-84-2	Phenothiazine	S	Y	NICEATM	Sigma-Aldrich	≥98%	1 of 1	No Cat	CO = 0							
566	Phenylbutazone	50-33-9	Aryl| Pyrazolidinedione/ Pyrazolidone	S	Y	LNS	Sigma-Aldrich	≥98.5%	1 of 1	No Cat	CO = 0							
567	Phenylephrine hydrochloride	61-76-7	Alcohol| Aliphatic Amine, secondary| Phenol	S	Y	ZEBET	Fisher Scientific	99%	1 of 1	No Cat	CO = 0							
568	Phenylthiourea	103-85-5	Aryl| Thiourea derivatives	S	Y	ZEBET	Sigma-Aldrich	≥98%	1 of 1	No Cat	CO = 0							
569	Piperazine	110-85-0 (18833-13-1 reported in ZEBET, which corresponds to Acetylline piperazinate)	Piperazine| Saturated heterocyclic amine| Saturated heterocyclic fragment	S	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
570	Potassium tetrafluoroborate	14075-53-7	Inorganic Salt	S	Y	ECETOC	Sigma-Aldrich	96%	1 of 1	No Cat	CO = 0							
571	Potato starch	56780-58-6	N/A	S	Y	ZEBET	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
572	Silicic acid (neat)	1343-98-2	N/A	S	Y	NICEATM	Sigma-Aldrich	99.9%	1 of 1	No Cat	CO = 0							
573	Sodium tripolyphosphate (Grade E, anhydrous) (10 mg)	7758-29-4	N/A	S	Y	NICEATM	Sigma-Aldrich	≥98%	1 of 1	No Cat	CO = 0						10 mg dose	
574	Tetrabromobisphenol A (1 of 2)	79-94-7	Aryl halide| Phenol	S	Y	NICEATM	Sigma-Aldrich	97%	1 of 2	No Cat	CO = 0							
575	Theobromine	83-67-0	N/A	S	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
576	Theophylline sodium (neat)	3485-82-3	Dihydropurinedione| Urea derivatives	S	Y	ZEBET	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
577	Theophylline sodium acetate	8002-89-9	N/A	S	Y	ZEBET	TCI	≥98%	1 of 1	No Cat	CO = 0							
578	Thiencarbazone-methyl	317815-83-1	Allyl| Amidine| Carboxylic acid ester| Ether| Hydrazone| Imide| Lactam| Sulfonamide| Sulfonyl urea| Thiophene	S	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	No Cat	CO = 0							
579	Tris(2-ethylhexyl)-4,4',4''-(1,3,5-triazine-2,4,6-triyltrilimino) tribenzoate	88122-99-0	Alkane, branched with tertiary carbon| Aromatic amine| Aryl| Carboxylic acid ester| Melamine	S	Y	EURL ECVAM	Proprietary	>98%	1 of 1	No Cat	CO = 0							?
580	Trisodium mono-(5-(1,2-dihydroxyethyl)-4-oxido-2-oxo-2,5-dihydro-furan-3-yl) phosphate	66170-10-3	Dihydroxyl group| Enol| Furanone/ Furanondione| Phosphate ester	S	Y	EURL ECVAM	Sigma-Aldrich	≥95%	1 of 1	No Cat	CO = 0							
581	Xanthinol nicotinate	437-74-1	Alcohol| Aliphatic Amine, tertiary| Aryl| Carboxylic acid| Fused unsaturated heterocycles| Pyridine| Pyrimidine derivatives| Urea derivatives	S	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 1	No Cat	CO = 0							
582	5-Chloro-2,4-disulphamoyl chloroacetanilide	Unknown	N/A	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
583	C10 alpha-Olefins (neat)	68855-58-3	Allyl	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
584	C16 alpha-Olefin (neat)	68855-58-3	Allyl	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
585	Cerium-2-ethylhexanoate	24593-34-8 (other possible CAS # may be 7435-02-1 and 56797-01-4)	Carboxylic acid	Unknown	N	ZEBET	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
586	iso-Tridecanal	61497-46-9	Aldehyde| Isopropyl	Unknown	N	ZEBET	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
587	Silan 165 (Chemical name: 3,3,11,11-Tetramethoxy-2,12-dioxa-7-thia-3,11-disilatridecane)	29055-11-6	AlkoxySilane| Sulfide	Unknown	N	ZEBET	Unknown	Unknown	1 of 1	No Cat	CO = 0							?
588	2,2-Dimethylbutanoic acid	595-37-9	Carboxylic acid	L	Y	ECETOC	Sigma-Aldrich	96%	1 of 1	SCNM (Cat 1)	CO mean ≥ 1; Conj mean ≥ 2	6/6; 6/6	**Possibly CO pers D21** (at least)	at least 1/6			Study terminated on D14 with CO = 3 in 1/6, CO = 2 in 2/6, CO = 1 in 3/6, IR = 2 in 1/6, IR = 1 in 1/6, IR = 0 in 4/6, CR = 1 in 1/6, CR = 0 in 5/6 and CC = 0 in 6/6; Possibly CO irreversible	X
589	iso-Butanol (2 of 2)	78-83-1	Alcohol| Isopropyl	L	Y	ZEBET	Sigma-Aldrich	≥99%	2 of 2	SCNM (Cat 1)	Conj mean ≥ 2; CO mean ≥ 1	3/3; 2/3	**Possibly CO pers D21** (at least)	1/3			Delayed effects; Study terminated on D14 with CO = 3 in 1/3, CO = 0 in 2/3, IR = 0 in 3/3, CR = 1 in 1/3, CR = 0 in 2/3, and CC = 0 in 3/3; CO fully reversible by D14 in 1/3 and by D1 in 1/3; D7 not recorded; Possibly CO irreversible	X
590	Triton X-100 (neat) (3 of 3)	9002-93-1	Alcohol| Alkane branched with quaternary carbon| Aryl| Ether| tert-Butyl	L	Y	NICEATM	Sigma-Aldrich	laboratory grade	3 of 3	SCNM (Cat 1)	CO mean ≥ 1	3/3	**Possibly CO pers D21** (at least)	1/3			Delayed effects; Study terminated on D14 with CO = 3 in 1/3, CO = 0 in 2/3, IR = 1 in 3/3, CR = 1 in 1/3, CR = 0 in 2/3, CC = 2 in 1/3 and CC = 0 in 2/3; Possibly CO irreversible	
591	Benzyl alcohol (10%)	100-51-6	Alcohol| Benzyl	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	99.8%	1 of 1	SCNM (Cat 1)	CO mean ≥ 1	3/3	**Possibly CO pers D21** (at least)	1/3			Delayed effects; Study terminated on D14 with CO = 3, IR = 1, CR = 3 and CC = 2 in 1/3 and all other animals fully reversed by D9 or earlier; Possibly CO irreversible	X
592	Dibutyltin dilaurate	77-58-7	Carboxylic acid| Tin, organo	L	Y	NICEATM	Sigma-Aldrich	95%	1 of 1	SCNM (Cat 1)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	**Possibly Conj pers D21**	2/3			Study terminated on D14 with CO = 0 in 3/3, IR = 0 in 3/3, CR = 3 in 2/3, CR = 0 in 1/3, CC = 4 in 1/3, CC = 3 in 1/3 and CC = 0 in 1/3; 1 animal fully reversed by D14; Possibly Conj irreversible	X
593	Surfonic N-95 (Chemical name: Nonyl phenol ethoxylate, branched)	9016-45-9	Alcohol| Benzyl| Ether	L	Y	NICEATM	Huntsman	100%	1 of 1	SCNM (Cat 1)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 5/6	Conj pers D7; CO pers D7; IR pers D7	5/6; 4/6; 1/6			Study terminated on D14 with CO = 2 in 1/6, CO = 1 in 1/6, IR = 1 in 1/6, CR = 2 in 1/6, and CC = 3 in 1/6; 1 animal fully reversed by D7; 3 animals fully reversed by D14	X
594	Surfonic N-85 (Chemical name: Nonyl phenol ethoxylate, branched)	9016-45-9	Alcohol| Benzyl| Ether	L	Y	NICEATM	Unknown	Unknown	1 of 1	SCNM (Cat 1)	IR mean ≥ 1; CO mean ≥ 1; Conj mean ≥ 2	6/6; 5/6; 5/6	Conj pers D7; CO pers D7; IR pers D7	6/6; 4/6; 2/6			Study terminated on D14 with CO = 2 in 3/6, IR = 1 in 1/6, CR = 1 in 6/6, CC = 2 in 4/6 and CC = 1 in 1/6	X

Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
595	Chlorendic anhydride	115-27-5	Acid anhydride| Alkenyl halide| Alkyl halide| Bridged-ring carbocycles| Fused saturated heterocycles| Oxolane| Saturated heterocyclic fragment	S	Y	NICEATM	Sigma-Aldrich	97%	1 of 1	SCNM (Cat 1)	IR mean ≥ 1; Conj mean ≥ 2	5/6; 4/6	Conj pers D7; IR pers D7; CO pers D7	5/6; 4/6; 2/6			Study terminated on D14 with CO = 2 in 3/6, CO = 1 in 2/6, IR = 1 in 4/6, CR = 1 in 5/6, CC = 2 in 1/6 and CC = 1 in 4/6	X
596	Iso-Decylglucoside	Unknown	N/A	Unknown	N	ZEBET	Unknown	Unknown	1 of 1	SCNM (Cat 1)	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	CO pers D7; Conj pers D7	3/3; 3/3			Delayed effects; Study terminated on D14 with CO = 2, CR = 2 and CC = 2 or 1 in 2/3; 1 animal fully reversed by D14	X
597	Methyl phosphonic acid bis (oxiranylmethyl) ester	77375-34-9 (77275-34-9 reported in ZEBET, which is wrong)	N/A	Unknown	N	ZEBET	Unknown	Unknown	1 of 1	SCNM (Cat 1)	CO mean ≥ 1; Conj mean ≥ 2	2/3; 2/3	CO pers D7; Conj pers D7; IR pers D7	1/3; 1/3; 1/3			Study terminated on D14 with CO = 2 in 1/3; 1 animals fully reversed by D7; CO = 0 on D2 in 1/3	X
598	Sodium hydrogenated tallow L-glutamine	Unknown	N/A	Unknown	N	NICEATM	Unknown	Unknown	1 of 1	SCNM (Cat 1)	CO mean ≥ 1	3/3	CO pers D7; Conj pers D7; IR pers D7	1/3; 1/3; 1/3			Study terminated on D14 with CO = 2, IR = 1, CR = 1 and CC = 1 in 1/3	X
599	Alcohol SDA 39C (95%)	64-17-5 (Ethanol) 84-66-6 (Diethylphthalate)	Ethanol	L	Y	NICEATM	Fisher Scientific; PHARMCO-AAPER	Unknown	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	CO pers D7; Conj pers D7	1/3; 1/3			Study terminated on D10 with CR = 2 and CC = 1 in 1/3; 2 animals fully reversed by D7 SDA = special denatured alcohol (99.01% (v/v) Ethanol + 0.99% (v/v) Diethylphthalate)	X
600	alpha-Hexyl cinnamic aldehyde (5% in Alcohol SDA 39C)	101-86-0	Alpha,beta unsaturated aldehyde| Benzyl	L	Y	NICEATM	Sigma-Aldrich (for alpha-Hexyl cinnamic aldehyde); Fisher Scientific (for Alcohol SDA 39C)	≥95%	1 of 1	SCNM (Cat 2A or higher)	Conj mean ≥ 2; CO mean ≥ 1	3/3; 2/3	CO pers D7; Conj pers D7	2/3; 2/3			Study terminated on D10 with CO = 1 in 2/3, CR = 2 in 2/3, CC = 2 in 1/3 and CC = 1 in 1/3; 1 animal fully reversed by D4 SDA = special denatured alcohol (99.01% (v/v) Ethanol + 0.99% (v/v) Diethylphthalate)	X
601	Emulphogene BC-610 (Chemical name: Polyoxyethylene (12) Tridecyl Ether)	78330-21-9	Alcohol| Alkoxy| Ether	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 5/6	CO pers D7; Conj pers D7; IR pers D7	6/6; 6/6; 5/6			Study terminated on D7	X
602	Ethanol (neat) (4 of 4)	64-17-5	Alcohol	L	Y	NICEATM	Sigma-Aldrich	>99.8%	4 of 4	SCNM (Cat 2A or higher)	CO mean ≥ 1	2/3	CO pers D7; Conj pers D7	2/3; 1/3			Study terminated on D14 with CO = 1 in 2/3; CO = 0 on D2 in 1/3; 1 animal fully reversed by D5	X
603	Furfuryl alcohol	98-00-0	Alcohol| Allyl| Aryl| Furane	L	Y	ECETOC	Sigma-Aldrich	≥98	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; IR mean ≥ 1	1/1; 1/1	CO pers D7; Conj pers D7	1/1; 1/1			One single animal fully reversed by D14; Observations indicating irritation	X
604	Igepal CA-720 (Chemical name: Octyl phenol ethoxylate, branched)	9036-19-5 or 9002-93-1 (9016-45-9 reported in NICEATM ALTTOX, which is wrong)	Alcohol| Alkane branched with quaternary carbon| Aryl| Ether| tert-Butyl	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	6/6; 6/6; 6/6	CO pers D7; Conj pers D7; IR pers D7	6/6; 6/6; 4/6			Study terminated on D7	X
605	Igepal CO-720 (Chemical name: Nonyl phenol ethoxylate, branched)	68412-54-4 or 9016-45-9 or 26027-38-3 (9016-45-9 reported in NICEATM ALTOX)	Alcohol| Benzyl| Ether	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2	6/6; 6/6	CO pers D7; Conj pers D7; IR pers D7	6/6; 6/6; 5/6			Study terminated on D7	X
606	Isazofos (Cheminal name: O-(5-Chlor-1-isopropyl-1,2,4-triazol-3-yl)-O,O-diethylthiophosphate)	42509-80-8	Alkoxy| Aryl halide| Isopropyl| Thiophosphate	L	Y	NICEATM	SCBT	>98%	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 2/3; 2/3	CO pers D7	3/3			Study terminated on D14 with CO = 1 in 1/3; 2 animals fully reversed by D14	X
607	Polysolvan (Chemical name: n-Butyl glycolate)	7397-62-8	Alcohol| Carboxylic acid ester	L	Y	ZEBET	Sigma-Aldrich	≥90%	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3	CO pers D7; Conj pers D7; IR pers D7	1/3; 1/3; 1/3			Delayed effects; Study terminated on D7 with CO = 3, IR = 1, CR = 2 and CC = 1 in 1/3; 2 animals fully reversed by D7	X
608	Silan 253 (Chemical name: 3-(Triethoxysilyl)-N,N-bis-3-(triethoxysilyl)-propyl-propane-1-amine)	18784-74-2	Aliphatic Amine, tertiary| Alkoxy| Alkoxysilane	L	Y	ZEBET	Fluorochem	100%	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3	CO pers D7; Conj pers D7	2/3; 2/3			At least 2/3 for CO, CR and CC persistence on D7; Study terminated on D4 in 1/3 and on D7 in 2/3	X
609	Sodium lauryl ether sulphate (unknown concentration)	3088-31-1	Alkoxy| Ether| Sulfate	L	N	ZEBET	Unknown	Unknown	1 of 1	SCNM (Cat 2A or higher)	Conj mean ≥ 2	5/6	Conj pers D7	5/6			Study terminated on D7	X
610	Cetylpyridinium chloride (1%)	6004-24-6	Ammonium salt| Aryl| Pyridine	L (tested in solvent, available as S)	Y	NICEATM	Sigma-Aldrich	>99%	1 of 1	SCNM (Cat 2A or higher)	Conj mean ≥ 2; CO mean ≥ 1	3/3; 2/3	Conj pers D7; CO Pers D7	3/3; 2/3			Study terminated on D14 with CO = 1 in 1/3; CO = 0 on D2 in 1/3; CO = 0 on D8 in 1/3; 1 animal fully reversed by D9; 1 animal fully reversed by D10	X
611	Aluminium sulphate hydrate	17927-65-0 (10043-01-3 reported in NICEATM ALTTOX, which corresponds to Aluminium sulphate)	N/A	S	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2	at least 5/6; 5/6	CO pers D7; Conj pers D7	6/6; 6/6			Study terminated on D7; 10 mg dose	X
612	Ethoxyphenylenediamine	1197-37-1	Alkoxy| Ether| Precursors quinoid compounds	S	N	NICEATM	Unknown	Unknown	1 of 1	SCNM (Cat 2A or higher)	Conj mean ≥ 2; IR mean ≥ 1	3/3; 2/3	Conj pers D7; CO pers D7	2/3; 1/3			Study terminated on D14 with CR = 1 and CC = 2 in 1/3, with CO fully reversing on D14 and IR fully reversing on D7; CR fully reversed in the other two animals on day 7 and day 14; CC fully reversed in the other two animals on day 7 in both animals; CO fully reversed in the other two animals on day 2 and day 7; IR fully reversed in the other two animals on day 3 and day 7	X
613	n-Butyl carbamate	592-35-8	Carbamate	S	Y	ZEBET	Sigma-Aldrich	98%	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	CO pers D7; Conj pers D7	3/3; 3/3			Study terminated on D7	X
614	o-Phenylenediamine (1 of 2)	95-54-5	Precursors quinoid compounds	S	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 2	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	Conj pers D7; CO pers D7; IR pers D7	3/3; 1/3; 1/3			Study terminated on D7	X
615	o-Phenylenediamine (2 of 2)	95-54-5	Precursors quinoid compounds	S	Y	NICEATM	Sigma-Aldrich	≥99%	2 of 2	SCNM (Cat 2A or higher)	CO mean ≥ 1	2/3	CO pers D7; Conj pers D7; IR pers D7	2/3; 2/3; 1/3			Study terminated on D14 with CO = 1 in 1/3, CR = 1 in 2/3 and CC = 2 in 1/3; 1 animal fully reversed by D7	X
616	Sodium lauryl sulphate (neat)	151-21-3	Alkoxy| Sulfate	S	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1	2/3	Conj pers D7	1/3			Study terminated on D14 with CR = 1 in 1/3; 1 animal fully reversed by D3; 1 animal fully reversed by D6	X
617	Sodium pyrosulphite (Sodium disulphite)	7681-57-4	N/A	S	Y	ZEBET	Sigma-Aldrich	98-100.5%	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	CO pers D7; Conj pers D7; IR pers D7	3/3; 3/3; 3/3			Study terminated on D7; Delayed effects	X
618	Sucrose fatty acid ester (neat)	Unknown	N/A	S	N	NICEATM	Unknown	Unknown	1 of 1	SCNM (Cat 2A or higher)	CO mean ≥ 1	2/3	CO pers D7; Conj pers D7; IR pers D7	2/3; 1/3; 1/3			Study terminated on D14 with CO = 1 in 1/3; CO = 0 in the whole study in 1/3; CO = 0 on D8 in 1/3; 1 animal fully reversed by D2; 1 animal fully reversed by D8	X
619	1-Piperidinecarboxaldehyde	2591-86-8	Formylamino| Piperidine| Saturated heterocyclic amine| Saturated heterocyclic fragment	L	Y	NICEATM	Sigma-Aldrich	99%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2	6/6; 6/6					Study terminated on D3	X
620	2,2,3-Trimethyl-3-cyclo-pentene-1-acetaldehyde	4501-58-0	Allyl| Cycloalkene| Ketone	L	Y	ZEBET	Parchem	85-100%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1	2/3					Study terminated on D4 or D7 (unclear); May be Cat 2A based on CO and/or CR persistence on D7 in 2/3 (unclear if data reports do D7 or D4)	X
621	2,3-Dibromopropanol	96-13-9	Alcohol| Alkyl halide	L	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2	6/6; 5/6					Study terminated on D3	X
622	3-Cyclohexene-1-methanol	1679-51-2	Alcohol| Alkane, branched with tertiary carbon| Allyl| Cycloalkene	L	Y	ZEBET	Sigma-Aldrich	98%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3					Study terminated on D3	X
623	Diethylenetriamine-pentaacetic acid pentasodium salt (unknown concentration; assumed to be ~40%, aqueous)	140-01-2	Aliphatic Amine, tertiary| Carboxylic acid	L	Y	ZEBET	Sigma-Aldrich	purum; ~40%, aqueous	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2	2/3; 2/3					Study terminated on D3	X
624	Methyl trifluoroacetate	431-47-0	Alkyl halide| Carboxylic acid ester	L	Y	NICEATM	Sigma-Aldrich	99%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; IR mean ≥ 1	5/6; 5/6					Study terminated on D3	X
625	Parafluoroaniline	371-40-4	Aniline| Aryl halide	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2	6/6; 6/6					Study terminated on D3	X
626	Iso-Cyanic acid polymethylene polyphenylene ester	9016-87-9	Benzyl| Isocyanate	L	Y	NICEATM	Sigma-Aldrich	Unknown	1 of 1	SCNM (Cat 2 or Cat 1)	Conj mean ≥ 2	4/6					Study terminated on D3	X
627	Toluene (2 of 2)	108-88-3	Aryl	L	Y	NICEATM	Sigma-Aldrich	≥99.9%	2 of 2	SCNM (Cat 2 or Cat 1)	Conj mean ≥ 2	4/6					Study terminated on D3	X
628	Toluene diisocyanate	26471-62-5	Aryl| Isocyanate	L	Y	NICEATM	Merck	Unknown	1 of 1	SCNM (Cat 2 or Cat 1)	Conj mean ≥ 2	6/6					Study terminated on D3	X
629	1,2-Dodecanediol	1119-87-5	Dihydroxyl group	S	Y	ZEBET	Sigma-Aldrich	90%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; IR mean ≥ 1	3/3; 3/3					Study terminated on D3	X
630	3-Mercapto-1,2,4-triazole	3179-31-5	Aryl| Thiourea derivatives| Triazole	S	Y	ZEBET	Sigma-Aldrich	97%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3					Study terminated on D3	X
631	6-Methyl Purine	2004-03-7	Purine derivatives	S	Y	NICEATM	Sigma-Aldrich	≥99%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1	6/6					Study terminated on D3	X
632	Hyton (Chemical name: 2-Amino-5-phenyl-1,3-oxazol-4(5H)-one)	2152-34-3	Amidine| Aryl| Lactams| Oxazolidine derivatives| Saturated heterocyclic fragment	S	Y	ZEBET	Sigma-Aldrich	≥98%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2	3/3; 3/3					Study terminated on D3; Available in Sigma under product number P0048	X
633	Iminodiacetic acid	142-73-4	Sarcosine	S	Y	ZEBET	Sigma-Aldrich	≥98%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3					Study terminated on D3	X
634	L-Aspartic acid	56-84-8	Alpha amino acid| Carboxylic acid	S	Y	ECETOC / ZEBET	Sigma-Aldrich	≥99%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; IR mean ≥ 1	2/3; 2/3					Study terminated on D3; Two studies are reported in ECETOC and ZEBET with the exact same animal scores and are considered duplicate entries	X
635	L-Glutamic acid HCL	138-15-8	Alpha amino acid| Carboxylic acid	S	Y	ZEBET	Sigma-Aldrich	>99%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	2/3; 2/3; 2/3					Study terminated on D3	X
636	Nicotinamide	98-92-0	Aryl| Carboxamide| Pyridine	S	Y	ZEBET	Sigma-Aldrich	≥99.5%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3					Study terminated on D3	X
637	Potassium hexacyanoferrate II	14459-95-1	N/A	S	Y	ZEBET	Sigma-Aldrich	≥99.5%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1	2/3					Study terminated on D3	X
638	Potassium hexacyanoferrate III	13746-66-2	N/A	S	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1	3/3					Study terminated on D3	X
639	TPBP C4 Amide (Chemical name: Phosphonium, triphenylphenyl-methyl-, salt with 1,1,2,2,3,3,4,4,4 -nonafluoro-N-methyl-1 butanesulfonamide (1:1))	332350-93-3	N/A	S	Y	NICEATM	Unknown	Unknown	1 of 1	SCNM (Cat 2 or Cat 1)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3					Study terminated on D3 with CO = 2 in 3/3	X

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Study Number	Test Chemical Name	CAS RN	Organic Functional Groups	Physical Form as tested	Physical Form Confirmation e.g., by MSDS (Y / N)	Data Source	Commercial Source	Available Purity	Number of Studies	UN GHS Classification	Drivers of Classification						Comments	Should Not Be Used
											Severity		Persistence		Specific Observations			
											Cut-off values	Number of animals	Cut-off time	Number of animals	CO = 4 or other observations	Number of animals		
640	4,4-Diphenylmethane diisocyanate	101-68-8	Benzyl| Isocyanate	S	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	SCNM (Cat 2 or Cat 1)	Conj mean ≥ 2; IR mean ≥ 1	5/6; at least 4/6					Study terminated on D3	X
641	Potassium cyanate	590-28-3	N/A	S	Y	ECETOC / ZEBET	Sigma-Aldrich	96%	1 of 1	SCNM (Cat 2 or Cat 1)	Conj mean ≥ 2	3/3					Study terminated on D3; Two studies are reported in ECETOC and ZEBET with the exact same animal scores and are considered duplicate entries	X
642	Sodium silicate (2.4 ratio hydrous)	1344-09-8	N/A	S	Y	NICEATM	PQ Corporation; Samarth Chemical Products	Unknown	1 of 1	SCNM (Cat 2 or Cat 1)	Conj mean ≥ 2	5/6					Study terminated on D3; 10 mg dose	X
643	Thiazolium, 3-ethyl-2-[3-(3-ethyl-2-thiazolidinylidene)-1-propenyl]-4,5-dihydro-iodide	3065-71-2	Ammonium salt| Conjugated system| Saturated heterocyclic fragment| Sulfide| Thiazolidine| Thiazoline| Unsaturated heterocyclic fragment	S	Y	NICEATM	Unknown	Unknown	1 of 1	SCNM (Cat 2 or Cat 1)	Conj mean ≥ 2	3/3					Study terminated on D2 due to extreme chemosis in all animals (score 4); For all other endpoints only D1 scores available	X
644	Diacetone alcohol	123-42-2	Alcohol| Ketone	L	Y	LNS	Sigma-Aldrich	99%	1 of 1	SCNM (Cat 2A)	CO mean ≥ 1; Conj mean ≥ 2	3/3; 2/3	CO pers D7	1/3			Original study indicates a CO = 1 in 1/3 on D14; However, study comment states full reversibility on D14; Most likely, it was meant as D21	X
645	Poly(ethylene glycol) butyl ether	9004-77-7	Alcohol| Alkoxy| Ether	L	Y	ZEBET	Sigma-Aldrich	Unknown	1 of 1	SCNM (Cat 2A)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 2/3	Conj pers D7; CO Pers D7	2/3; 1/3			Study terminated on D7	X
646	p-Ethyltoluene	622-96-8	Aryl	L	Y	NICEATM	Sigma-Aldrich	≥95%	1 of 1	SCNM (Cat 2A)	Conj mean ≥ 2	4/6	Conj pers D7	4/6			Study terminated on D7 with CR = 3 in 1/6, CR = 2 in 2/6, CR = 1 in 1/6 and CC = 1 in 2/6; 1 animal fully reversed by D4; 1 animal fully reversed by D7	X
647	Triton X-100 (5%) (2 of 2)	9002-93-1	Alcohol| Alkane branched with quaternary carbon| Aryl| Ether| tert-Butyl	L	Y	ECETOC	Sigma-Aldrich	laboratory grade	2 of 2	SCNM (Cat 2A)	CO mean ≥ 1; Conj mean ≥ 2	5/6; 4/6	Conj pers D7	4/6			Study terminated on D7 with CC = 1 in 1/6; 1 animal fully reversed by D3, 1 animal fully reversed by D7 and 3 animals fully reversed by D10	
648	p-Anisidine	104-94-9	Aniline| Ether	S	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 1	SCNM (Cat 2A)	CO mean ≥ 1; Conj mean ≥ 2; IR mean ≥ 1	3/3; 3/3; 3/3	Conj pers D7; CO Pers D7	3/3; 2/3			Study terminated on D7	X
649	Maneb	12427-38-2	Thiocarbamate	S	Y	ECETOC	Sigma-Aldrich	analytical standard	1 of 1	SCNM (Cat 2A)	Conj mean ≥ 2	6/6	Conj pers D7	2/6			Study terminated on D7 with CR = 1 in 1/6 and with CR and CC = 1 in 1/6; 4 animals fully reversed by D7	X
650	1,2,3-Trimercaptopropane	4756-13-2	Thioalcohol	L	Y	ECETOC	Unknown	Unknown	1 of 1	SCNM (Cat 2)	Conj mean ≥ 2	2/3					Study terminated on D3 with CC = 1 in 1/6 and with CR and CC = 1 in 1/6; 1 animal fully reversed by D2	X
651	Chlorhexidine HCL	3697-42-5	Aryl halide| Guanidine	S	Y	ZEBET	Sigma-Aldrich	≥98%	1 of 1	SCNM (Cat 2)	Conj mean ≥ 2	2/3					Study terminated on D3	X
652	Dodecanal (1% in Alcohol SDA 39C)	112-54-9	Aldehyde	L	Y	NICEATM	Sigma-Aldrich (for Dodecanal); Fisher Scientific (for Alcohol SDA 39C)	≥95%	1 of 1	SCNM (Cat 2B)	Conj mean ≥ 2	2/2					2 animals only, both fully reversed by D7 SDA = special denatured alcohol (99.01% (v/v) Ethanol + 0.99% (v/v) Diethylphthalate)	X
653	1,2-Expoxydodecane	2855-19-8	Epoxide| Saturated heterocyclic fragment	L	Y	ZEBET	Alfa Aesar	95%	1 of 1	SCNM (No Cat)	CO > 0 **	** CO 1/3					Study terminated on D3	X
654	1-Methoxy-2-propanol	107-98-2	Alcohol| Ether	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	SCNM (No Cat)	CO > 0 **	** CO 2/6; Conj 2/6					Study terminated on D8 with CO = 1 in 2/6, CR = 2 in 1/6 and CR = 1 in 4/6	X
655	Butyl alcohol	78-92-2	Alcohol	L	Y	NICEATM	Sigma-Aldrich	≥99.5%	1 of 1	SCNM (No Cat)	CO > 0 **	** CO 2/6; Conj 2/6					Animal 6 killed on D7 without explanation with CO = 3, IR = 2 and CR = 2; 3 animals fully reversed by D7; 2 animals fully reversed by D14	X
656	Carsonon N-6 (5%) (Chemical name: Nonyl phenol ethoxylate, branched)	9016-45-9 (127087-87-0 reported in NICEATM ALTTOX, which corresponds to Tergitol NP nonionic surfactants)	Alcohol| Benzyl| Ether	L	Y	NICEATM	Unknown	Unknown	1 of 1	SCNM (No Cat)	CO > 0 **	** CO 1/6; IR 1/6					Study terminated on D7 with CO = 2 and CR = 1 in 1/6; 3 animals fully reversed by D3; 2 animals fully reversed by D4	X
657	Diepoxide 126 (Chemical name: 3,4-Epoxycyclohexylmethyl 3,4-epoxycyclohexane carboxylate)	2386-87-0	Alkane, branched with tertiary carbon| Carboxylic acid ester| Cycloalkane| Fused saturated heterocycles| Saturated heterocyclic fragment	L	Y	ZEBET	Sigma-Aldrich	Unknown	1 of 1	SCNM (No Cat)	CO > 0 **	** CO 1/3					Study terminated on D3	X
658	n-Butyl glycidyl ether	2426-08-6	Alkoxy| Epoxide| Ether| Saturated heterocyclic fragment	L	Y	NICEATM	Sigma-Aldrich	97%	1 of 1	SCNM (No Cat)	CO > 0 **	** CO 2/6; Conj 2/6; IR 1/6					Study terminated on D3	X
659	Silan 103 (Chemical name: Trimethoxypropylsilane)	1067-25-0	AlkoxySilane	L	Y	ZEBET	Sigma-Aldrich	97%	1 of 1	SCNM (No Cat)	CO > 0 **	** CO 1/3; Conj 1/3					Study terminated on D3	X
660	Ammonium persulphate	7727-54-0	N/A	S	Y	ZEBET	Sigma-Aldrich	≥98%	1 of 1	SCNM (No Cat)	CO > 0 **	** CO 1/3					Study terminated on D3	X
661	Fomesafen, acid form	72128-02-0	Alkyl halide| Aryl| Aryl halide| Benzamide| Ether| Sulfonamide	S	Y	ECETOC	Unknown	Unknown	1 of 1	SCNM (No Cat)	CO > 0 **	** CO 1/6					Study terminated on D7 with CR = 1 in 1/6 and with CC = 1 in 1/6; 1 animal fully reversed by D2; 3 animals fully reversed by D7; Fomesafen (CAS # 72178-02-0) available from Sigma	X
662	1,5-Dimethyl cyclo-octadiene	3760-14-3	Allyl| Cycloalkene	L	Y	ECETOC	Unknown	Unknown	1 of 1	SCNM (No Cat)	CO > 0						Study terminated on D7 with CR = 1 in 1/6; 4 animals fully reversed by D2; 1 animal fully reversed by D7	X
663	alpha-Lactid	4511-42-6	Dioxane| Lactone| Saturated heterocyclic fragment	S	Y	ZEBET	Sigma-Aldrich	98%	1 of 1	SCNM (No Cat)	CO > 0						Study terminated on D4	X
664	Dibromoneopentyl glycol	3296-90-0	Alcohol| Alkane branched with quaternary carbon| Alkyl halide	S	Y	NICEATM	Sigma-Aldrich	98%	1 of 1	SCNM (No Cat)	CO > 0						Study terminated on D8 with CR = 1 in 2/6	X
665	L-Lysine monohydrate	39665-12-8	Aliphatic Amine, primary| Alpha amino acid	S	Y	ZEBET	Sigma-Aldrich	≥98%	1 of 1	SCNM (No Cat)	CO > 0						Study terminated on D3	X
666	Sodium cyanate	917-61-3	N/A	S	Y	ZEBET	Sigma-Aldrich	96%	1 of 1	SCNM (No Cat)	CO > 0						Study terminated on D3	X
667	2,4-Difluoronitrobenzene	446-35-5	Aryl halide| Nitrobenzene	L	Y	ECETOC	Sigma-Aldrich	99%	1 of 1	SCNM (No Cat)	CO = 0 **	** Conj 2/6					Study terminated on D7 with CR = 1 in 1/6; 5 animals fully reversed by D7	X
668	Ethylbutanal	97-96-1	Aldehyde	L	Y	ZEBET	VWR	98%	1 of 1	SCNM (No Cat)	CO = 0 **	** Conj 1/3; IR 1/3					Study terminated on D7	X
669	Tripropylene glycol monomethyl ether	25498-49-1	Alcohol| Ether	L	Y	NICEATM	Sigma-Aldrich	≥97.5%	1 of 1	SCNM (No Cat)	CO = 0 **	** IR 2/6; Conj 1/6					Study terminated on D3	X
670	C12-16 blend alpha olefin	Unknown	N/A	L	N	NICEATM	Unknown	Unknown	1 of 1	SCNM (No Cat)	CO = 0						Study terminated on D3 with CR = 1 in 4/6; RTECS # AZ7987000	X
671	C6 alpha-Olefin	68855-57-2	N/A	L	N	NICEATM	Unknown	Unknown	1 of 1	SCNM (No Cat)	CO = 0						Study terminated on D3 with CR = 1 in 2/6	X
672	Ethoxyquin	91-53-2	Alkoxy| Allyl| Dihydroquinoline/ Dihydroisoquinoline| Ether	L	Y	EURL ECVAM	Sigma-Aldrich	analytical standard	1 of 1	SCNM (No Cat)	CO = 0						Study terminated on D3 with CR = 1 in 1/6	X
673	iso-Myristyl alcohol	5333-48-2	Alcohol| Alkane, branched with tertiary carbon	L	Y	ECETOC	Sigma-Aldrich	Unknown	1 of 1	SCNM (No Cat)	CO = 0						Study terminated on D3 with CR = 1 in 1/3; 1 animal fully reversed by D1; 1 animal fully reversed by D2	X
674	Polymethylenepolyphenylenepolyamine	25214-70-4	N/A	L	Y	NICEATM	Unknown	Unknown	1 of 1	SCNM (No Cat)	CO = 0						Study terminated on D3 with CR = 1 in 2/6	X
675	Tergitol nonionic surfactant min-foam 2x (Alcohols,C11-15-secondary, ethoxylated propoxylated)	68551-14-4	N/A	L	Y	NICEATM	Dow	100%	1 of 1	SCNM (No Cat)	CO = 0						Study terminated on D3 with CR = 1 in 3/4; Tergitol® min foam 1x (CAS # 68551-14-4) available from Sigma	X
676	Sodium sulphite	7757-83-7	N/A	S	Y	ZEBET	Sigma-Aldrich	≥98%	1 of 1	SCNM (No Cat)	CO = 0						Study terminated on D3	X
677	Tetrabromobisphenol A (2 of 2)	79-94-7	Aryl halide| Phenol	S	Y	NICEATM	Sigma-Aldrich	97%	2 of 2	SCNM (No Cat)	CO = 0						Study terminated on D3 with CR = 1 in 3/6	
678	Silan 167 (Chemical name: Trimethoxy-[3-(3-trimethoxysilylpropyldisulfanyldisulfanyl)propyl]silane)	41453-78-5	AlkoxySilane| Sulfide, poly	Unknown	N	ZEBET	Unknown	Unknown	1 of 1	SCNM (No Cat)	CO = 0						Study terminated on D3; CR = 1 on D3 in 1/3	X
679	Diethyl phthalate	84-66-2	Aryl| Carboxylic acid ester	L	Y	NICEATM	Sigma-Aldrich	99.5%	1 of 1	SCNM (No Cat)	NA						Data only for D1 with CR = 1 in 2/6	X
680	Anisole	100-66-3	Aryl| Ether	L	Y	ZEBET	Sigma-Aldrich	≥99%	1 of 1	SCNM	Conj mean ≥ 2	1/1	CO pers D7; Conj pers D7	1/1; 1/1			1 single animal; Study terminated on D7; CO, CR and CC = 2 on D7	X
681	Dow Corning Siloxanes and Silicones, DI-Me (35% aq dispersion) (Chemical name: Polydimethylsiloxane)	63148-62-9	Silane	L	Y	NICEATM	SCBT	100%	1 of 1	SCNM	IR mean ≥ 1	1/2					2 animals only, 1 fully reversed by D3 and the other fully reversed by D4; 1 animal with IR > 1	X