Table 11.3. The IC50s for test substances, relative controls and positive controls at laboratory C in the SIRC-CVS:TEA validation phase III study

Chemical Code	Chemical Code in Laboratory C	Test Sbstance (IC50 ug/mL)			Relative Control (IC50 ug/mL)			Positive Control (IC50 ug/mL)		
		Run 1	Run 2	Mean	Run 1	Run 2	Mean	Run 1	Run 2	Mean
P3-002	**SC72**	>2500	>2500	>2500	1628.00	1753.10	1690.55	126.10	123.50	124.80
P3-003*2	**SC61**	>2500	>2500	>2500	1177.80	1413.70	1295.75	87.50	102.00	94.75
P3-004	**SC74**	105.80	244.30	175.05	1085.20	1618.10	1351.65	123.80	126.50	125.15
P3-005*2	**SC62**	>5000	>5000	>5000	1256.90	1375.10	1316.00	109.00	119.60	114.30
P3-006	**SC77**	845.80	1302.60	1074.20	1248.60	1555.90	1402.25	129.50	126.00	127.75
P3-007	**SC79**	77.40	35.40	56.40	1181.10	1747.40	1464.25	136.50	129.90	133.20
P3-009	**SC80**	>2500	>2500	>2500	1256.90	1665.80	1461.35	109.00	111.90	110.45
P3-010*2	**SC63**	3464.60	2748.70	3106.65	1831.10	1108.60	1469.85	120.60	87.50	104.05
P3-011	**SC81**	<39.1	<39.1	<39.1	1285.60	1418.20	1351.90	180.80	137.30	159.05
P3-012*2	**SC64**	3210.00	2765.90	2987.95	1851.80	1415.30	1633.55	117.10	119.50	118.30
P3-013	**SC82**	>5000	>5000	>5000	1186.40	1123.90	1155.15	125.70	140.60	133.15
P3-014	**SC83**	>5000	>5000	>5000	1400.10	1064.40	1232.25	114.80	133.40	124.10
P3-015	**SC84**	328.00	218.10	273.05	1071.90	1250.00	1160.95	141.60	133.20	137.40
P3-016	**SC85**	<39.1	40.40	<40.4	1017.50	1013.80	1015.65	140.10	130.60	135.35
P3-017	**SC87**	>2500	>2500	>2500	1353.90	1365.50	1359.70	123.70	138.30	131.00
P3-018	**SC88**	>5000	>5000	>5000	1154.10	1269.40	1211.75	116.70	121.10	118.90
P3-019*2	**SC65**	285.10	246.00	265.55	1159.40	1913.30	1536.35	121.20	118.80	120.00
P3-020*2	**SC66**	1946.00	2991.20	2468.60	1864.20	1573.00	1718.60	129.60	113.20	121.40
P3-021	**SC90**	<39.1	39.80	<39.8	1115.00	1166.50	1140.75	120.20	143.20	131.70
P3-023	**SC91**	-	-	-	-	-	-	-	-	-
P3-024*2	**SC68**	172.90	55.30	114.10	1182.30	1678.20	1430.25	136.10	90.90	113.50
P3-025	**SC92**	>5000	>5000	>5000	1017.10	1112.30	1064.70	137.20	124.90	131.05
P3-026	**SC93**	<39.1	<39.1	<39.1	1674.10	1106.50	1390.30	120.20	129.00	124.60
P3-028*2	**SC69**	<39.1	<39.1	<39.1	1822.50	1787.80	1805.15	116.70	82.60	99.65
P3-029*2	**SC70**	55.70	33.20	44.45	1786.40	1433.90	1610.15	128.00	113.90	120.95
P3-030	**SC97**	<19.5	<19.5	<19.5	1061.00	1169.40	1115.20	124.90	136.40	130.65
P3-031	**SC89**	85.90	86.50	86.20	1259.60	1112.60	1186.10	111.50	123.10	117.30

Chemical Code	Chemical Code in Laboratory C	Test Sbstance (IC50 ug/mL)			Relative Control (IC50 ug/mL)			Positive Control (IC50 ug/mL)		
		Run 1	Run 2	Mean	Run 1	Run 2	Mean	Run 1	Run 2	Mean
P3-032	**SC98**	41.70	55.90	48.80	1279.50	1369.20	1324.35	123.90	129.10	126.50
P3-033*2	**SC67**	>5000	>5000	>5000	1133.00	1794.70	1463.85	114.70	83.90	99.30
P3-034	**SC71**	>2500	>2500	>2500	1244.80	1743.90	1494.35	141.30	98.90	120.10
P3-035	**SC73**	103.30	184.50	143.90	1269.40	1754.20	1511.80	105.90	109.20	107.55
P3-036	**SC75**	931.40	940.20	935.80	1418.20	1676.30	1547.25	148.00	119.40	133.70
P3-037	**SC76**	>2500	>2500	>2500	1389.20	1181.20	1285.20	114.00	122.70	118.35
P3-038	**SC78**	1786.60	2253.10	2019.85	1070.70	1288.20	1179.45	121.60	119.00	120.30
P3-039	**SC95**	919.10	922.50	920.80	1286.30	1143.10	1214.70	126.80	131.70	129.25
P3-040	**SC96**	62.50	56.20	59.35	1173.40	1116.60	1145.00	134.00	123.10	128.55
P3-041	**SC99**	<39.1	<39.1	<39.1	1456.50	1159.60	1308.05	138.80	146.30	142.55
P3-044	**SC86**	3114.80	2076.00	2595.40	1801.20	1154.50	1477.85	118.40	127.20	122.80
P3-091	**SC94**	<39.1	<39.1	<39.1	1356.10	1241.50	1298.80	129.10	135.60	132.35
P3-092	**SC100**	149.60	443.10	296.35	1193.80	1143.70	1168.75	119.00	121.40	120.20

*1; Each IC50 of test substances, relative controls and positive controls was expressed as an average every set.

*2; Ten test substances were shared in Laboratory A, B and C.

*3: -; Inapplicable

Table 12. Inter-laboratory reproducibility of the SIRC-CVS:TEA method in the phase II study

Chemical code	Name of test substance	Laboratory A	Laboratory B	Laboratory C	Inter-laboratory reproducibility
P2-001	Piperonylbutoxide	P	P	P	1
P2-002	2,5-dimethylhexaediol	N	N	N	1
P2-003	1-(2-propoxy-1-methylethoxy)-2-propanol	N	N	N	1
P2-004	ammonium nitrate	P	P	P	1
P2-005	potassium tetrafluoroborate	N	N	N	1
P2-006	3,4,4'-trichlorocarbanilide	P	P	P	1
P2-007	1-bromohexane	P	P	P	1
P2-008	4,4'-methylenebis(2,6-di-tert-butylphenol)	N	N	N	1
P2-009	propylene glycol propyl ether	N	N	N	1
P2-010	ethyl thioglycolate	P	P	P	1
P2-011	sodium oxalate	P	P	P	1
P2-012	2-phospho-L-ascorbic acid trisodium salt	N	N	N	1
P2-013	1-bromo-4-chlorobutane	P	P	P	1
P2-014	sodium hydrogensulfite	P	P	P	1
P2-015	Isobutyraldehyde	P	P	P	1
P2-016	1-naphthaleneacetic acid	P	P	P	1
P2-017	propyl 4-hydroxybenzoate	P	P	P	1
P2-018	ethyl 2,6-dichloro-5-fluoro-beta-oxo-3-pyridinepro	P	P	P	1
P2-019	Camphene	P	P	P	1
P2-020	Cyclopentanol	N	N	N	1

*1: N; Negative, P; Positive

*2: 1; All laboratories' judge agreed.

Table 13. Inter-laboratory reproducibility of the SIRC-CVS:TEA method in the phase III study

Chemical code	Name of test substance	Laboratory A	Laboratory B	Laboratory C	Inter-laboratory reproducibility
P3-003	dipropyl disulfide	P	P	N	0
P3-005	2-(2-ethoxyethoxy)ethanol	N	N	N	1
P3-010	n,n-dimethylguanidine sulfate	N	P	N	0
P3-012	polyethylene hydrogenated caster oil (40E.O.)	N	P	N	0
P3-019	diethyl toluamide	P	P	P	1
P3-020	4-nitrobenzoic acid	N	N	N	1
P3-024	2-amino-3-hydroxy pyridine	P	P	P	1
P3-028	tetraethylene glycol	P	P	P	1
P3-029	dodecanoic acid	P	P	P	1
P3-033	gamma-butyrolactone	N	N	N	1

*1: N; Negative, P; Positive

*2: 1; All laboratories' judge agreed, 0; Only two laboratories' judge agreed

Table 14. Eye irritation potential of test substances in the SIRC-CVS:TEA validation phase III study

Chemical code	Laboratory	Name of test substance	Run 1	Run 2	Final Evaluation
P3-001	B	2-ethoxyethyl methacrylate	P	P	P
P3-002	C	iso-octylthioglycolate	N	N	N
P3-003	A/B/C	dipropyl disulfide	P/P/N	P/P/N	P
P3-004	C	1-bromo-octane	P	P	P
P3-005	A/B/C	2-(2-ethoxyethoxy)ethanol	N/N/N	N/N/N	N
P3-006	C	dioctyl ether	P	P	P
P3-007	C	3-phenoxybenzyl alcohol	P	P	P
P3-008	B	glycidyl methacrylate	P	P	P
P3-009	C	2-ethylhexylthioglycolate	N	N	N
P3-010	A/B/C	n,n-dimethylguanidine sulfate	N/P/N	N/P/N	N
P3-011	C	6-hydroxy-2,4,5-triaminopyrimidine Sulfate	P	P	P
P3-012	A/B/C	polyethylene hydrogenated caster oil (40E.O.)	N/P/N	N/P/N	N
P3-013	C	2,2'-methylene-bis-(6-(2Hbenzotriazol-2-yl)-4-	N	N	N
P3-014	C	cellulose 2-(2-hydroxy-3-(trimethylammonio)propoxy	N	N	N
P3-015	C	3,4-dimethoxy benzaldehyde	P	P	P
P3-016	C	3-chloropropionitrile	P	P	P
P3-017	C	2-methyl-1-pentanol	N	N	N
P3-018	C	ethyl-2-methylacetoacetate	N	N	N
P3-019	A/B/C	diethyl toluamide	P/P/P	P/P/P	P
P3-020	A/B/C	4-nitrobenzoic acid	N/N/N	N/N/N	N
P3-021	C	sodium chloroacetate	P	P	P
P3-022	A	2,4,11,13-tetraazatetra (Chlorohexidine glucocinat	P	P	P
P3-023	C	-	-	-	-
P3-024	A/B/C	2-amino-3-hydroxy pyridine	P/P/P	P/P/P	P
P3-025	C	sodium benzoate	N	N	N
P3-026	C	methylthioglycolate	P	P	P
P3-027	A	3-(2-aminoethylamino)propyl]trimethoxysilane	P	P	P
P3-028	A/B/C	tetraethylene glycol	P/P/P	P/P/P	P
P3-029	A/B/C	dodecanoic acid	P/P/P	P/P/P	P

Chemical code	Laboratory	Name of test substance	Run 1	Run 2	Final Evaluation
P3-030	C	1,2-benzisothiazol-3(2H)-one	P	P	P
P3-031	C	2-hydroxy-1,4-naphthoquinone	P	P	P
P3-032	C	disodium 4,4'-bis(2-sulfonatostyryl)biphenyl	P	P	P
P3-033	A/B/C	gamma-butyrolactone	N/N/N	N/N/N	N
P3-034	C	1-methylpropyl benzene	N	N	N
P3-035	C	4-(methylmercapto)benzaldehyde	P	P	P
P3-036	C	1,9-decaine	P	P	P
P3-037	C	2,4-dimethyl-3-pentanol	N	N	N
P3-038	C	1-ethyl-3-methylimidazolium ethylsulfate	N	N	N
P3-039	C	1,2,4-triazole,sodium salt	P	P	P
P3-040	C	4,4'-(4,5,6,7-tetrabromo-1,1-dioxido-3H-2,1-benzox	P	P	P
P3-041	C	benzenamine,4,4'-(4-aimino-3-methylphenyl)(4-imino	P	P	P
P3-042	A	1-(9H-carbozol-4-yloxy)-3-[[2-(2-methoxy phenoxy)e	P	P	P
P3-043	B	3-methyl-1,5-di(2,4-xylyl)-1,3,5-Triazapenta-1,4-d	P	P	P
P3-044	C	isopropyl acetoacetate	N	N	N
P3-045	A	(3R,4R)-4-acetoxy-3-[(R)-(tert-butyldimethylsilylo	P	P	P
P3-046	B	1-octanol	P	P	P
P3-047	B	2-benzyloxyethanol	N	N	N
P3-048	B	butanol	N	N	N
P3-049	B	isobutyl alcohol	P	P	P
P3-050	B	isopropyl alcohol	N	N	N
P3-051	B	myristyl alcohol	P	P	P
P3-052	B	hexyl cinnamic aldehyde	P	P	P
P3-053	B	n-butanal	P	P	P
P3-054	B	monoethanolamine	P	P	P
P3-055	B	m-phenylenediamine	P	P	P
P3-056	B	ethyl acetate	N	N	N
P3-057	B	isopropyl myristate	N	N	N
P3-058	B	methoxyethyl acrylate	P	P	P
P3-059	B	methyl acetate	N	N	N
P3-060	B	methyl cyanoacetate	N	N	N

Chemical code	Laboratory	Name of test substance	Run 1	Run 2	Final Evaluation
P3-061	B	imidazole	P	P	P
P3-062	B	pyridine	N	N	N
P3-063	B	isopropyl bromide	N	N	N
P3-064	B	cyclohexanone	N	N	N
P3-065	B	2-methylbutyric acid	N	N	N
P3-066	B	-	-	-	-
P3-067	B	citric acid	P	P	P
P3-068	B	potassium sorbate	N	N	N
P3-069	B	sodium salicylate	N	N	N
P3-070	B	distearyldimethylammonium chloride	P	P	P
P3-071	B	n-lauroylsarcosine sodium salt	P	P	P
P3-072	B	sodium lauryl sulfate	P	P	P
P3-073	A	triton X-100 (5%)	P	P	P
P3-074	A	2-ethylhexyl p-dimethyl-amino benzoate	P	P	P
P3-075	A	promethazine hydrochloride	P	P	P
P3-076	A	2-ethyl-1-hexanol	P	P	P
P3-077	A	3-methoxy-1.2-propanediol	N	N	N
P3-078	A	cyclohexanol	N	N	N
P3-079	A	ethanol	N	N	N
P3-080	A	n-hexanol	N	N	N
P3-081	A	3,3-dimethylpentane	P	P	P
P3-082	A	methyl cyclopentane	P	P	P
P3-083	A	toluene	N	N	N
P3-084	A	acetone	N	N	N
P3-085	A	gluconolactone	N	N	N
P3-086	A	methyl amyl ketone (2-heptanol)	N	N	N
P3-087	A	methyl ethyl ketone (2-butanone)	N	N	N
P3-088	A	methyl isobutyl ketone(4-methyl 2-pentanol)	N	N	N
P3-089	A	glycerol	N	N	N
P3-090	A	cetylpyridinium bromide	P	P	P
P3-091	C	triton X-100	P	P	P

Chemical code	Laboratory	Name of test substance	Run 1	Run 2	Final Evaluation
P3-092	C	tween20	P	P	P
P3-093	A	sodium hydroxide	P	P	P
P3-094	A	glycolic acid	N	N	N
P3-095	A	3,3-dithiodipropionic acid	N	N	N
P3-096	A	sucrose fatty acid ester	P	P	P
P3-097	A	methyl para-Hydroxybenzoate	P	P	P
P3-098	A	silic acid	P	P	P
P3-099	A	benzyl alcohol	N	N	N
P3-100	A	lactic acid	N	N	N

*1: N; Negative, P; Positive

*2: Eye irritaion potential of common test substances were expressed as a representative of three laboratories.

*3: -; Inapplicable

Table 15. List of the test substances used in the phase II and phase III studies of SIRC-CVS:TEA validation and their *in vitro* judgments[#]

Code No.	Chemical Name	CAS No.	Physi-cality	Molecular Weight	Purity	Supplier	Water solubility	Log D	Vapor Pressure	Source	Final Chemical Class	INCI Listing	GHS	EPA	*In vitro* Judgment
Pase II Study															
P2-001	Piperonylbutoxide	51- 03- 6	Liquid	338.44	90	Sigma-Aldrich	0.021	4.75	5.31E-07	US-EPA 8	Ether	INCI	No	III	Positive
P2-002	2,5-dimethylhexaediol	110-03-2	Solid	146.23	97	Sigma-Aldrich	13	0.76	4.37E-03	STE review	Alcohol	No	1	I	Negative
P2-003	1-(2-propoxy-1-methylethoxy)-2-propanol	29911-27-1	Liquid	176.25	≥98.5	Sigma-Aldrich	72	0.8	7.48E-04	STE review	Alcohol, Ether	INCI	2	III	Negative
P2-004	ammonium nitrate	6484-52-2	Solid	80.04	≥98	Sigma-Aldrich	-	-	-	NICEATM 6	Inorganic salt	INCI	2	III	Positive
P2-005	potassium tetrafluoroborate	14075-53-7	Solid	125.9	96	Sigma-Aldrich	-	-	-	ECETOC 71	Inorganic salt, Halogen compound	No	No	IV	Negative
P2-006	3,4,4'-trichlorocarbanilide	101-20-2	Solid	315.58	99	Sigma-Aldrich	1.00E-04	6.07	8.89E-06	Cosing 36	Amide, Halogen compound	INCI	No	IV	Positive
P2-007	1-bromohexane	111-25-1	Liquid	165.07	≥98.0	Sigma-Aldrich	0.069	3.85	5.33E-01	STE review	Halogen compound	No	No	IV	Positive
P2-008	4,4'-methylenebis(2,6-di-tert-butylphenol)	118-82-1	Solid	424.66	98	Sigma-Aldrich	3.60E-05	8.97	6.13E-10	ECETOC 26	Phenol compound	No	No	IV	Negative
P2-009	propylene glycol propyl ether	1569-01-3	Liquid	118.17	99	Sigma-Aldrich	99	0.68	1.22E-01	NICEATM 1	Alcohol, Ether	INCI	2	II	Negative
P2-010	ethyl thioglycolate	623-51-8	Liquid	120.17	97	Sigma-Aldrich	13	1.1	3.60E-01	NICEATM 13	Thiol compound, Ester	INCI	No	III	Positive
P2-011	sodium oxalate	62-76-0	Solid	134	≥99.5	Sigma-Aldrich	-	-	-	ECETOC 14	Organic salt	INCI	1	I	Positive

Code No.	Chemical Name	CAS No.	Physi-cality	Molecular Weight	Purity	Supplier	Water solubility	Log D	Vapor Pressure	Source	Final Chemical Class	INCI Listing	GHS	EPA	*In vitro* Judgment
P2-012	2-phospho-L-ascorbic acid trisodium salt	66170-10-3	Solid	322.05	≥95.0	Sigma	-	-	-	BASF 6	Heterocyclic compound, Organic salt, Phosphorus compound	INCI	No	III	Negative
P2-013	1-bromo-4-chlorobutane	6940-78-9	Liquid	171.46	99	Sigma-Aldrich	0.29	2.75	3.45E-01	STE review	Halogen compound	No	No	IV	Positive
P2-014	sodium hydrogensulfite	7631-90-5	Solid	104.06	≥58.5	Sigma-Aldrich	-	-	-	NICEATM 17	Inorganic salt	INCI	No	III	Positive
P2-015	Isobutyraldehyde	78-84-2	Liquid	72.11	98	Sigma-Aldrich	15	0.76	1.96E+01	STE review	Aldehyde	INCI	2	III	Positive
P2-016	1-naphthaleneacetic acid	86-87-3	Solid	186.21	≥95.0	Wako Pure	120	-0.14	4.17E-07	ECETOC 12	Carboxylic acid, Polycyclic compound	No	1	I	Positive
P2-017	propyl 4-hydroxybenzoate	94-13-3	Solid	180.2	≥98.0	Sigma-Aldrich	1.2	2.88	1.24E-04	LNS 1	Ester, Phenol	INCI	No	III	Positive
P2-018	ethyl 2,6-dichloro-5-fluoro-beta-oxo-3-pyridinepropionate	96568-04-6	Solid	294.11	98	Sigma-Aldrich	0.19	1.84	6.09E-06	NICEATM 10	Halogen compound, Heterocyclic compound, Ester, Ketone	No	2	III	Positive
P2-019	Camphene	79-92-5	Solid	136.23	95	Sigma-Aldrich	0.011	4.24	4.51E-01	STE review	Hydrocarbon	INCI	2	III	Positive
P2-020	Cyclopentanol	96-41-3	Liquid	86.13	99	Sigma-Aldrich	85	0.75	3.29E-01	ECETOC 57	Alcohol	No	2	II	Negative
Pase III Study															
P3-001	2-ethoxyethyl methacrylate	2370-63-0	Liquid	158.19	99	Sigma-Aldrich	17	1.44	1.08E-01	ECETOC 31	Methacrylate, Ester, Ether	No	No	IV	Positive
P3-002	iso-octylthioglycolate	25103-09-7	Liquid	204.33	≥98.0	Wako Pure	-	-	-	ECETOX 32	Thio compound, Ester	INCI	No	IV	Negative
P3-003	dipropyl disulfide	629-19-6	Liquid	150.31	98	Sigma-Aldrich	2.1	4.19	9.80E-02	STE review	Disulfide compound	No	No	IV	Positive
P3-004	1-bromo-octane	111-83-1	Liquid	193.12	99	Sigma-Aldrich	0.011	4.87	0.45	STE review	Halogen compound	No	No	IV	Positive

Code No.	Chemical Name	CAS No.	Physi-cality	Molecular Weight	Purity	Supplier	Water solubility	Log D	Vapor Pressure	Source	Final Chemical Class	INCI Listing	GHS	EPA	*In vitro* Judgment
P3-005	2-(2-ethoxyethoxy)ethanol	111-90-0	Liquid	134.17	≥99	Sigma-Aldrich	590	-0.42	9.77E-03	Cosing 25	Alcohol, Ether	INCI	No	III	Negative
P3-006	dioctyl ether	629-82-3	Liquid	242.44	99	Sigma-Aldrich	5.80E-03	7.15	-	Cognis 14	Ether	INCI	No	IV	Positive
P3-007	3-phenoxybenzyl alcohol	13826-35-2	Liquid	200.23	98	Sigma-Aldrich	0.19	3.39	2.95E-07	NICEATM 11	Alcohol	No	No	III	Positive
P3-008	glycidyl methacrylate	106-91-2	Liquid	142.15	97	Sigma-Aldrich	17	0.34	-	STE review	Methacrylate, Ester	No	No	III	Positive
P3-009	2-ethylhexylthioglycolate	7659-86-1	Liquid	204.33	≥95.0	Sigma-Aldrich	0.13	3.99	8.88E-04	ECETOC 52	Thiol compound, Ester	No	No	IV	Negative
P3-010	n,n-dimethylguanidine sulfate	598-65-2	Solid	272.33	97	Sigma-Aldrich	-	-	-	STE review	Organic salt	No	No	III	Negative
P3-011	6-hydroxy-2,4,5-triaminopyrimidine Sulfate	1603-02-7	Solid	239.21	≥95.0	Wako Pure	679	-4.86	-	Cosing 32	Heterocyclic compound(salt)	No	No	IV	Positive
P3-012	polyethylene hydrogenated caster oil (40E.O.)	61788-85-0	Solid	About 400	-	Sigma-Aldrich	-		-	STE review	Surfactant (nonionic)	INCI	No	IV	Negative
P3-013	2,2'-methylene-bis-(6-(2Hbenzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol)	103597-45-1	Solid	658.87	99	Sigma-Aldrich	3.70E-08	14.32	1.51E-25	Ciba 7	Phenol, Heterocyclic compound	No	No	IV	Negative
P3-014	cellulose, 2-(2-hydroxy-3-(trimethylammonio)propoxy) ethyl ether chloride	68610-92-4	Solid	>257	-	Sigma-Aldrich	-	-	-	J&J 2	Quaternary ammonium compound, Synthetic polymer	INCI	No	III	Negative
P3-015	3,4-dimethoxy benzaldehyde	120-14-9	Solid	166.17	99	Sigma-Aldrich	1.6	1.37	4.88E-04	NICEATM 16	Aldehyde	No	No	III	Positive
P3-016	3-chloropropionitrile	542-76-7	Liquid	89.52	≥98.0	Wako Pure	23	0.29	1.44E-01	ECETOC 58	Halogen compound, Nitrile compound	No	2	III	Positive
P3-017	2-methyl-1-pentanol	105-30-6	Liquid	102.17	99	Sigma-Aldrich	12	1.70	2.23E-01	STE review	Fatty alcohol	No	2	III	Negative

Code No.	Chemical Name	CAS No.	Physi-cality	Molecular Weight	Purity	Supplier	Water solubility	Log D	Vapor Pressure	Source	Final Chemical Class	INCI Listing	GHS	EPA	*In vitro* Judgment
P3-018	ethyl-2-methylacetoacetate	609-14-3	Liquid	144.17	90	Sigma	23	0.72	9.15E-02	STE review	Ester, Ketone	No	2	III	Negative
P3-019	diethyl toluamide	134-62-3	Liquid	191.27	95	Sigma-Aldrich	7.5	2.42	1.80E-04	US-EPA 2	Amide	INCI	2	III	Positive
P3-020	4-nitrobenzoic acid	62-23-7	Solid	167.12	≥98.0	Sigma-Aldrich	999	-1.22	1.17E-06	NICEATM 9	Carboxylic acid	No	2	III	Negative
P3-021	sodium chloroacetate	3926-62-3	Solid	116.48	98	Sigma-Aldrich	-	-	-	STE review	Organic salt, Halogen Compound	No	2	III	Positive
P3-022	2,4,11,13-tetraazatetra (Chlorohexidine glucocinate)	18472-51-0	Liquid	897.76	-	Wako Pure	-	-	-	NICEATM 2	Organic salt, Halogen Compound	INCI	2	II	Positive
P3-023	3,3-dithiodipropionic acid	1119-62-6	Solid	210.27	≥97.0	Wako Pure	1000	-3.36	1.64E-09	Kato (2013)	Carboxylic acid, Thio compound	No	2	II	-
P3-024	2-amino-3-hydroxy pyridine	16867-03-1	Solid	110.11	98	Sigma-Aldrich	15	-0.44	2.33E-07	Cosing 14	Heterocyclic compound, Amine	INCI	2	III	Positive
P3-025	sodium benzoate	532-32-1	Solid	144.1	≥99.0	Sigma-Aldrich	-	-	-	Cosing 18	Organic salt	INCI	2	II	Negative
P3-026	methylthioglycolate	2365-48-2	Liquid	106.14	95	Sigma-Aldrich	30	0.59	4.77E-01	ECETOC 1	Thio compound, Ester	INCI	1	II	Positive
P3-027	3-(2-aminoethylamino)propyl]trimethoxysilane	1760-24-3	Liquid	222.36	97	Chemos	1000	-2.33	8.21E-04	Evonik 1	Silicon compound	No	1	I	Positive
P3-028	tetraethylene glycol	17831-71-9	Liquid	302.32	-	Sigma-Aldrich	30	0.53	6.71E-07	TSCA	Acrylate, Ether, Ester	No	1	I	Positive
P3-029	dodecanoic acid	143-07-7	Solid	200.32	≥99	Sigma-Aldrich	16	2.56	8.81E-05	ECETOC 8	Fatty acid	INCI	1	I	Positive
P3-030	1,2-benzisothiazol-3(2H)-one	2634-33-5	Solid	151.18	≥97.0	Wako Pure	0.56	1.95	-	Cosing 5	Heterocyclic compound, Thio compound, Amide	INCI	1	I	Positive
P3-031	2-hydroxy-1,4-naphthoquinone	83-72-7	Solid	174.15	97	Sigma-Aldrich	31	-0.74	4.60E-06	Cosing 23	Phenol compound	INCI	2	III	Positive

Code No.	Chemical Name	CAS No.	Physi-cality	Molecular Weight	Purity	Supplier	Water solubility	Log D	Vapor Pressure	Source	Final Chemical Class	INCI Listing	GHS	EPA	*In vitro* Judgment
P3-032	disodium 4,4'-bis(2-sulfonatostyryl) biphenyl	27344-41-8	Solid	562.56	≥98.0	Wako Pure	-	-	-	Ciba 5	Sulfonic acid	INCI	1	I	Positive
P3-033	gamma-butyrolactone	96-48-0	Liquid	86.09	≥99	Sigma-Aldrich	70	-0.63	3.60E-02	STE review	Heterocyclic compound, Ketone	INCI	2	II	Negative
P3-034	1-methylpropyl benzene	135-98-8	Liquid	134.22	≥99	Wako Pure	0.011	4.09	2.27E-01	STE review	Hydrocarbon(aromatic)	No	No	IV	Negative
P3-035	4-(methylmercapto)benzaldehyde	3446-89-7	Liquid	152.21	95	Sigma-Aldrich	0.4	2.21	1.11E-03	ECETOX 38	Thio compound, Aldehyde	No	No	IV	Positive
P3-036	1,9-decaine	1647-16-1	Liquid	138.25	98	Sigma-Aldrich	6.40E-04	4.99	2.79E-01	STE review	Alkene	No	No	IV	Positive
P3-037	2,4-dimethyl-3-pentanol	3970-62-5	Liquid	116.2	97	Sigma-Aldrich	8.8	1.96	3.77E-01	STE review	Fatty alcohol	No	No	III	Negative
P3-038	1-ethyl-3-methylimidazolium ethylsulfate	342573-75-5	Liquid	236.29	99	Alfa Aesar	-	-	-	Evonik 5	Heterocyclic compound, Inorganic salt	No	No	III	Negative
P3-039	1,2,4-triazole,sodium salt	41253-21-8	Solid	91.05	90	Sigma-Aldrich	-	-	-	ECETOC 9	Heterocyclic compound	No	1	I	Positive
P3-040	4,4'-(4,5,6,7-tetrabromo-1,1-dioxido-3H-2,1-benzoxathiole-3,3-diyl) bis[2,6-dibromophenol]	4430-25-5	Solid	986.55	85	Sigma-Aldrich	4.60E-03	9.72	7.93E-23	Coising 2	Halogen compound, Phenol, Sulfonic acid	INCI	1	I	Positive
P3-041	benzenamine,4,4'-(4-aimino-3-methylphenyl)(4-imino-3-methyl-2,5-cyclohexadien-1-ylidene) methyl-2-methy HCL	3248-91-7	Solid	365.9	-	Sigma-Aldrich	-	-	-	Cosing 3	Organic salt	INCI	1	I	Positive
P3-042	1-(9H-carbozol-4-yloxy)-3-[[2-(2-methoxy phenoxy)ethyl] amino]-2-propanol	72956-09-3	Solid	406.47	≥98	LKT. Labs,Inc	0.053	2.69	6.17E-19	Glaxo 14	Polycyclic compound, Alcohol	No	No	IV	Positive
P3-043	3-methyl-1,5-di(2,4-xylyl)-1,3,5-Triazapenta-1,4-dien	33089-61-1	Solid	293.41	97	LKT. Labs,Inc	2.20E-03	5.59	3.43E-09	US-EPA 17	Triazapentadien compound	No	No	IV	Positive
P3-044	isopropyl acetoacetate	542-08-5	Liquid	144.17	≥95.0	Wako Pure	23	0.72	9.15E-02	NICEATM 4	Ester, Ketone	No	2	III	Negative

Code No.	Chemical Name	CAS No.	Physi-cality	Molecular Weight	Purity	Supplier	Water solubility	Log D	Vapor Pressure	Source	Final Chemical Class	INCI Listing	GHS	EPA	*In vitro* Judgment
P3-045	(3R,4R)-4-acetoxy-3-[(R)-(tert-butyldimethylsilyloxy)ethyl]-2-azetidinone	76855-69-1	Solid	287.43	98	Sigma-Aldrich	0.4	2.37	3.43E-06	Glaxo 2	Silicon compound	No	2	II	Positive
P3-046	1-octanol	111-87-5	Liquid	130.23	≥98.0	Wako Pure	1.2	2.88	1.52E-02	STE review	Fatty alcohol	INCI	2	II	Positive
P3-047	2-benzyloxyethanol	622-08-2	Liquid	152.19	≥97.0	Wako Pure	26	1.11	1.19E-03	STE review	Alcohol, Ether	INCI	2	II	Negative
P3-048	Butanol	71-36-3	Liquid	74.12	≥99.0	Wako Pure	48	0.84	1.14E+00	STE review	Alcohol	INCI	1	I	Negative
P3-049	isobutyl alcohol	78-83-1	Liquid	74.12	≥99.0	Sigma-Aldrich	68	0.68	2.19E+00	STE review	Alcohol	No	1	I	Positive
P3-050	isopropyl alcohol	67-63-0	Liquid	60.1	≥99.9	Wako Pure	141	0.17	1.08E+01	STE review	Alcohol	INCI	2	III	Negative
P3-051	myristyl alcohol	112-72-1	Solid	214.39	≥97.0	Wako Pure	5.80E-04	5.93	1.96E-04	STE review	Fatty alcohol	INCI	2	III	Positive
P3-052	hexyl cinnamic aldehyde	101-86-0	Liquid	216.32	≥97.0	Wako Pure	0.039	4.87	9.29E-05	Kojima (2013)	Aldehyde	INCI	n.a.	n.a.	Positive
P3-053	n-butanal	123-72-8	Liquid	72.11	≥98.0	Wako Pure	14	0.91	1.28E+01	STE review	Aldehyde	No	2	III	Positive
P3-054	monoethanolamine	141-43-5	Liquid	61.08	≥99.0	Sigma-Aldrich	1000	-4.08	6.11E-02	Kojima (2013)	Alkanolamine	INCI	2	III	Positive
P3-055	m-phenylenediamine	108-45-2	Solid	108.14	>98.0	TCI	77	-0.19	4.28E-04	STE review	Amine	INCI	1	I	Positive
P3-056	ethyl acetate	141-78-6	Liquid	88.11	99.8	Sigma-Aldrich	39	0.79	1.49E+01	STE review	Ester	INCI	No	III	Negative
P3-057	isopropyl myristate	110-27-0	Liquid	270.45	≥95.0	Wako Pure	2.60E-03	7.25	4.39E-05	STE review	Ester	INCI	No	IV	Negative
P3-058	methoxyethyl acrylate	3121-61-7	Liquid	130.14	≥98.0	Wako Pure	59	0.51	4.83E-01	STE review	Acrylate, Ether, Ester	No	1	II	Positive
P3-059	methyl acetate	79-20-9	Liquid	74.08	99.5	Sigma-Aldrich	81.5	0.28	4.91E+01	STE review	Ester	INCI	2	II	Negative

Code No.	Chemical Name	CAS No.	Physi-cality	Molecular Weight	Purity	Supplier	Water solubility	Log D	Vapor Pressure	Source	Final Chemical Class	INCI Listing	GHS	EPA	*In vitro* Judgment
P3-060	methyl cyanoacetate	105-34-0	Liquid	99.09	99	Sigma-Aldrich	1000	-2.96	2.92E-02	STE review	Ester, Nitrile compound	No	2	II	Negative
P3-061	Imidazole	288-32-4	Solid	68.08	99	Sigma-Aldrich	228	-0.7	3.20E-03	STE review	Heterocyclic compound, Amine	INCI	1	I	Positive
P3-062	Pyridine	110-86-1	Liquid	79.1	≥99.0	Sigma-Aldrich	893	0.83	3.04E+00	STE review	Heterocyclic compound	No	1	I	Negative
P3-063	isopropyl bromide	75-26-3	Liquid	122.99	≥97.0	Wako Pure	1.8	2.16	2.73E+01	STE review	Halogen compound	No	No	IV	Negative
P3-064	Cyclohexanone	108-94-1	Liquid	98.14	99.8	Sigma-Aldrich	15	0.82	3.99E-01	STE review	Ketone, Hydrocarbon(cyclic)	No	No	III	Negative
P3-065	2-methylbutyric acid	116-53-0	Liquid	102.13	≥98	Sigma-Aldrich	1000	-1.14	7.39E-02	STE review	Carboxylic acid	No	1	I	Negative
P3-066	calcium thioglycolate trihydrate	5793-98-6	Solid	184.22	>94.0	TCI	-	-	-	STE review	Thio compound, Organic salt	No	1	I	
P3-067	citric acid	77-92-9	Solid	192.12	≥99.5	Sigma-Aldrich	999	-6.91	7.64E-06	Kojima (2013)	Carboxylic acid	INCI	n.a.	n.a.	Positive
P3-068	potassium sorbate	24634-61-5	Solid	150.22	≥98.0	Sigma-Aldrich	-	-	-	Kojima (2013)	Organic salt	INCI	n.a.	n.a.	Negative
P3-069	sodium salicylate	54-21-7	Solid	160.1	≥99.5	Wako Pure	-	-	-	STE review	Organic salt, Phenol	INCI	1	I	Negative
P3-070	Distearyldimethyl ammonium chloride	107-64-2	Solid	586.5	>95.0	TCI	-	-	-	STE review	Quaternary ammonium compound	INCI	1	I	Positive
P3-071	n-lauroylsarcosine sodium salt	137-16-6	Solid	293.38	≥95.0	Wako Pure	-	-	-	Kojima (2013)	Surfactant (anionic)	INCI	2	III	Positive
P3-072	sodium lauryl sulfate	151-21-3	Solid	288.38	≥95.0	Wako Pure	-	-	-	STE review	Surfactant (anionic)	INCI	2	III	Positive
P3-073	triton X-100 (5%)	9002-93-1	Liquid	324.41	-	Sigma-Aldrich	-	-	-	Kojima (2013)	Surfactant (nonionic)	INCI	2	III	Positive
P3-074	2-ethylhexyl p-dimethyl-amino benzoate	21245-02-3	Liquid	277.4	≥97.0	Wako Pure	4.70E-03	5.41	6.09E-07	STE review	PABA derivative	INCI	No	IV	Positive

Code No.	Chemical Name	CAS No.	Physi-cality	Molecular Weight	Purity	Supplier	Water solubility	Log D	Vapor Pressure	Source	Final Chemical Class	INCI Listing	GHS	EPA	*In vitro* Judgment
P3-075	promethazine hydrochloride	58-33-3	Solid	320.88	98	Sigma-Aldrich	-	-	-	STE review	Heterocyclic compound, Organic salt	No	1	I	Positive
P3-076	2-ethyl-1-hexanol	104-76-7	Liquid	130.23	≥98.0	Wako Pure	1.7	2.72	-	STE review	Fatty alcohol	No	2	II	Positive
P3-077	3-methoxy-1.2-propanediol	623-39-2	Liquid	106.12	>98.0	TCI	843	-0.94	-	STE review	Alcohol, Ether	No	No	IV	Negative
P3-078	Cyclohexanol	108-93-0	Liquid	100.16	≥95.0	Sigma-Aldrich	44	1.28	1.17E-01	STE review	Alcohol	No	1	I	Negative
P3-079	Ethanol	64-17-5	Liquid	46.068	≥99.5	Wako Pure	183	-0.18	1.10E+01	STE review	Alcohol	INCI	2	I	Negative
P3-080	n-hexanol	111-27-3	Liquid	102.17	≥99.0	Sigma-Aldrich	8.8	1.86	1.26E-01	STE review	Alcohol	INCI	2	II	Negative
P3-081	3,3-dimethylpentane	562-49-2	Liquid	100.2	99	Sigma-Aldrich	8.20E-03	4.02	1.02E+01	STE review	Hydrocarbon	No	No	IV	Positive
P3-082	methyl cyclopentane	96-37-7	Liquid	84.16	>96.0	TCI	0.084	3.17	1.67E+01	STE review	Hydrocarbon	No	No	III	Positive
P3-083	Toluene	108-88-3	Liquid	92.14	≥99.5	Wako Pure	0.32	2.72	3.69E+00	STE review	Hydrocarbon (aromatic)	INCI	2	III	Negative
P3-084	Acetone	67-64-1	Liquid	58.08	≥99.5	Sigma-Aldrich	94.7	-0.04	4.64E+01	STE review	Ketone	INCI	2	II	Negative
P3-085	Gluconolactone	90-80-2	Solid	178.14	≥97.0	Wako Pure	999	-3.47	1.01E-10	Kojima (2013)	Polyol	INCI	No	IV	Negative
P3-086	methyl amyl ketone (2-heptanol)	110-43-0	Liquid	114.19	≥98.0	Wako Pure	5.0	2	6.31E-01	STE review	Ketone	No	No	III	Negative
P3-087	methyl ethyl ketone (2-butanone)	78-93-3	Liquid	72.11	>99.0	TCI	47	0.47	1.53E+01	STE review	Ketone	INCI	2	III	Negative
P3-088	methyl isobutyl ketone(4-methyl 2-pentanol)	108-10-1	Liquid	72.11	≥99.0	Sigma-Aldrich	12	1.33	2.43E+00	STE review	Ketone	INCI	No	III	Negative
P3-089	Glycerol	56-81-5	Liquid	92.09	≥99.0	Wako Pure	715	-1.85	3.09E-05	STE review	Polyol	INCI	No	IV	Negative

Code No.	Chemical Name	CAS No.	Physi-cality	Molecular Weight	Purity	Supplier	Water solubility	Log D	Vapor Pressure	Source	Final Chemical Class	INCI Listing	GHS	EPA	*In vitro* Judgment
P3-090	cetylpyridinium bromide	140-72-7	Solid	384.44	≥97.0	Sigma-Aldrich	-	-	-	STE review	Surfactant (cationic)	No	1	I	Positive
P3-091	triton X-100	9002-93-1	Liquid	324.41	-	Sigma-Aldrich	-	-	-	STE review	Surfactant (nonionic)	INCI	1	I	Positive
P3-092	tween20	9005-64-5	Liquid	346.46	-	Sigma-Aldrich	-	-	-	STE review	Surfactant (nonionic)	INCI	No	III	Positive
P3-093	sodium hydroxide	1310-73-2	Solid	40	≥97.0	Wako Pure	-	-	-	STE review	Alkali	INCI	1	I	Positive
P3-094	glycolic acid	79-14-1	Solid	76.05	≥98.0	Sigma-Aldrich	1000	-4.62	-	Kato (2013)	Carboxylic acid	INCI	2	III	Negative
P3-095	3,3-dithiodipropionic acid	1119-62-6	Solid	210.27	≥97	Wako Pure	1000	-3.36	1.64E-09	NICEATM	Carboxilic acid, Thio compound	No	2	II	Negative
P3-096	sucrose fatty acid ester	Non	Solid	>342.3	-	TCI	-	-	-	STE review	Polyol, Ester		2	II	Positive
P3-097	methyl para-Hydroxybenzoate	99-76-3	Solid	152.15	≥99.0	Wako Pure	5.6	1.86	7.40E-04	Ohno(1999)	Ester, Phenol	INCI	2	II	Positive
P3-098	silic acid, dehydrogate	7699-41-4	Solid	78.1	-	Wako Pure	-	-	-	Ohno(1999)	Silicon compound	No	No	IV	Positive
P3-099	benzyl alcohol	100-51-6	Liquid	108.14	≥98.5	Sigma-Aldrich	47	1.06	2.11E-02	STE review	Alcohol	INCI	1	I	Negative
P3-100	lactic acid	50-21-5	Liquid	90.08	≥85.0	Wako Pure	1000	-4.2	2.00E-03	STE review	Carboxylic acid	INCI	1	I	Negative

#; The analysis was performed based on IC50 of triethanolamine in UN GHS classification system in a bottom-up approach.

Table 16. Overall analysis by the judgment based on IC_{50} value of Triethanolamine (TEA) in UN GHS classification system in a bottom-up approach and top-down approach

Regulatory System	Bottom-Up Approach	Top-Down Approach
Accuracy	54.8% (63/115)	53.9% (62/115)
Sensitivity	59.4% (41/69)	71.4% (20/28)
Specificity	47.8% (22/46)	48.3% (42/87)
False Negative Rate	40.6% (28/69)	28.6% (8/28)
False Positive Rate	52.2% (24/46)	51.7% (45/87)

Table 18.1. Analysis classified by chemical class (GHS, Bottom-up, TEA); Surfactant and Halogen compound

Regulatory System	Surfactant	Halogen compound
Accuracy	85.7% (6/7)	63.6% (7/11)
Sensitivity	100.0%(5/5)	100.0%(5/5)
Specificity	50.0% (1/2)	33.3% (2/6)
False Negative Rate	0.0% (0/5)	0.0% (0/5)
False Positive Rate	50.0% (1/2)	66.7% (4/6)

Table 18.2. Analysis classified by chemical class (GHS, Bottom-up, TEA); Heterocyclic compounds and phenol

Regulatory System	Heterocyclic compound	Phenol
Accuracy	75.0% (9/12)	71.4% (5/7)
Sensitivity	75.0% (6/8)	75.0% (3/4)
Specificity	75.0% (3/4)	66.7% (2/3)
False Negative Rate	25.0% (2/8)	25.0% (1/4)
False Positive Rate	25.0% (1/4)	33.3% (1/3)

Table 18.3. Analysis classified by chemical class (GHS, Bottom-up, TEA); Organic salt and thiol compound

Regulatory System	Organic salt	Thiol compound
Accuracy	77.8% (7/9)	57.1% (4/7)
Sensitivity	71.4% (5/7)	66.7% (2/3)
Specificity	100.0%(2/2)	50.0% (2/4)
False Negative Rate	28.6% (2/7)	33.3% (1/3)
False Positive Rate	0.0% (0/2)	50.0% (2/4)

Table 18.4. Analysis classified by chemical class (GHS, Bottom-up, TEA); Ester and hydrocarbon

Regulatory System	Ester	Hydrocarbon
Accuracy	55.6% (10/18)	50.0% (3/6)
Sensitivity	60.0% (6/10)	50.0% (1/2)
Specificity	50.0% (4/8)	50.0% (2/4)
False Negative Rate	40.0% (4/10)	50.0% (1/2)
False Positive Rate	50.0% (4/8)	50.0% (2/4)

Table 18.5. Analysis classified by chemical class (GHS, Bottom-up, TEA); Ether and carboxylic acid

Regulatory System	Ether	Carboxylic acid
Accuracy	40.0% (4/10)	28.6% (2/7)
Sensitivity	40.0% (2/5)	28.6% (2/7)
Specificity	40.0% (2/5)	(0/0)
False Negative Rate	60.0% (3/5)	71.4% (5/7)
False Positive Rate	60.0% (3/5)	0 .% (0/0)

Table 18.6. Analysis classified by chemical class (GHS, Bottom-up, TEA); Alcohol and ketone

Regulatory System	Alcohol	Ketone
Accuracy	33.3% (7/21)	44.4% (4/9)
Sensitivity	25.0% (4/16)	16.7% (1/6)
Specificity	60.0% (3/5)	100.0%(3/3)
False Negative Rate	75.0% (12/16)	83.3% (5/6)
False Positive Rate	40.0% (2/5)	0.0% (0/3)

Table 19.1. Analysis classified by state (GHS, Bottom-up, TEA); Liquid and solid

Regulatory System	Liquid	Solid
Accuracy	43.3% (29/67)	70.8% (34/48)
Sensitivity	40.5% (15/37)	81.3% (26/32)
Specificity	46.7% (14/30)	50.0% (8/16)
False Negative Rate	59.5% (22/37)	18.8% (6/32)
False Positive Rate	53.3% (16/30)	50.0% (8/16)

Table 19.2. Analysis after cut Molecular weight (180) (GHS, Bottom-up, TEA)

Regulatory System	Analysis after Cut mw ≥ 180	Analysis after Cut mw < 180
Accuracy	71.4% (30/42)	45.2% (33/73)
Sensitivity	95.2% (20/21)	43.8% (21/48)
Specificity	47.6% (10/21)	48.0% (12/25)
False Negative Rate	4.8% (1/21)	56.3% (27/48)
False Positive Rate	52.4% (11/21)	52.0% (13/25)