

# Attachment 3\_Chemicals used to assess within laboratory reproducibility, transferability and between laboratory reproducibility

Givaudan-ID	Name	EC3, Geo Mean ICCVAM database	Classification	ICCVAM List	Casati et al., List	SENS-IT-IV List	Study Phase	Source	Order Number	Batch Number	MW	Solvent	CAS-Nr	Formula	cLogP
From List published by Casati <i>et al.</i> , ATLA, 2009															
GR-87-1787	Oxazolone	0.0028	strong-extreme		x	x	Phase II	SIGMA	E0753	124K3690	217.22	DMSO	15646-46-5	C <sub>12</sub> H <sub>11</sub> NO <sub>3</sub>	1.9
GR-60-7989	2,4-Dinitrochlorobenzene	0.049	strong-extreme	x	x	x	Phase I	ALDRICH	237329	1420612 41409035	202.55	DMSO	97-00-7	C <sub>6</sub> H <sub>3</sub> ClN <sub>2</sub> O <sub>4</sub>	2.2
GR-87-1790	4-Phenylenediamine	0.11	strong-extreme	x	x	x	Phase II	ALDRICH	78429	1416291 41609223	108.14	DMSO	106-50-3	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	0.9
GR-82-2963	Cinnamic aldehyde	1.3	moderate		x	x	Phase II	GIVAUDAN	1500001	9000538811	132.16	DMSO	104-55-2	C <sub>9</sub> H <sub>8</sub> O	1.9
GR-01-1375	Isoeugenol	1.5	moderate	x	x	x	Phase II	GIVAUDAN	6237001	9000691084	164.20	DMSO	97-54-1	C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	2.4
GR-60-8400	tetramethylthiuramdisulfide	3.1	moderate		x	x	Phase II	FLUKA	87940	374481/1 12307426	296.54	DMSO	137-26-8	C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> S <sub>4</sub>	2.7
GR-60-7976	2-Mercaptobenzothiazole	2.5	moderate	x	x	x	Phase II	FLUKA	63720	014801/1 42506102	167.25	DMSO	149-30-4	C <sub>7</sub> H <sub>5</sub> NS <sub>2</sub>	2.4
GR-57-0251	Eugenol	10.1	weak	x	x	x	Phase II	GIVAUDAN	5002001	9000724417	164.20	DMSO	97-53-0	C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	2.1
GR-57-0143	Cinnamyl alcohol	21.0	weak	x	x	x	Phase II	GIVAUDAN	1173001	9000626366	134.18	DMSO	104-54-1	C <sub>9</sub> H <sub>10</sub> O	1.7
GR-60-3682	Glyoxal	0.7	strong-extreme		x	x	Phase II	SIGMA	128465	1414774 50909111	58.04	DMSO	107-22-2	C <sub>2</sub> H <sub>2</sub> O <sub>2</sub>	-0.6
GR-61-0358	4-nitrobenzylbromide	0.1	strong-extreme		x	x	Phase II	FLUKA	73170	249839 686	216.03	DMSO	100-11-8	C <sub>7</sub> H <sub>6</sub> BrNO <sub>2</sub>	2.8
GR-87-1796	Methyldibromo glutaronitrile	0.9 /1.9	moderate		x	x	Phase II	FLUKA	34392	1386163 12009244	265.93	DMSO	35691-65-7	C <sub>6</sub> H <sub>6</sub> Br <sub>2</sub> N <sub>2</sub>	2.3
GR-60-4237	Salicylic acid	12.2 (1)	non-sensitizer	x	x	x	Phase II	FLUKA	84210	puriss	138.12	DMSO	69-72-7	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	1.1
GR-60-0595	Sodium lauryl sulfate	false positive	non-sensitizer	x	x	x	Phase II	FLUKA	71727	371996/1 51998	288.38	DMSO	151-21-3	C <sub>12</sub> H <sub>25</sub> NaO <sub>4</sub> S	3.4
GR-60-2116	Lactic acid	Neg. (2)	non-sensitizer	x	x	x	Phase II	FLUKA	69775	1433079 41209P09	90.08	DMSO	50-21-5	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	-0.5
GR-60-0500	Glycerol	NC (> 100%)	non-sensitizer		x	x	Phase II	FLUKA	49780	364809/1 54097	92.09	DMSO	56-81-5	C <sub>3</sub> H <sub>8</sub> O <sub>3</sub>	-1.7
Added from ICCVAM performance standards for alternative endpoints in the LLNA (w/o metals) and not in ECCVAM List															
GR-60-8329	4-Methylaminophenol sulphate (METOL)	0.8	strong-extreme	x			Phase II	FLUKA	69749	1413786 20809206	221.23	H2O / 10	55-55-0	C <sub>7</sub> H <sub>11</sub> NO <sub>3</sub> S	1.4
GR-87-1788	(5-chloro)-Methylisothiazolinone	0.01	strong-extreme	x			Phase II	FLUKA	00344	1292199 54406084	149.60	H2O /50	2682-20-4	C <sub>4</sub> H <sub>4</sub> ClNOS	1.2
GR-57-0320	Hexyl cinnamic aldehyde	9.9	weak	x			Phase I	GIVAUDAN	1320001	9000763336	216.32	DMSO	101-86-0	C <sub>15</sub> H <sub>20</sub> O	4.2
GR-03-2037	Citral	9.8	weak	x			Phase I	GIVAUDAN	6560703	9000595485	152.23	DMSO	5392-40-5	C <sub>10</sub> H <sub>16</sub> O	2.9
GR-60-2407	Phenyl benzoate	13.6	weak	x			Phase II	ALDRICH	14,271-9	09157-508	198.22	DMSO	93-99-2	C <sub>13</sub> H <sub>10</sub> O <sub>2</sub>	2.9
GR-87-1799	Imidazolidinyl urea	24.0	weak	x			Phase II	SIGMA	I5133	048K0664	388.29	DMSO	39236-46-9	C <sub>11</sub> H <sub>16</sub> N <sub>8</sub> O <sub>8</sub>	-4.8
GR-60-6416	Ethylene glycol dimethacrylate	32.9	weak	x			Phase I	FLUKA	03808	373292/1 25397	198.22	DMSO	97-90-5	C <sub>10</sub> H <sub>14</sub> O <sub>4</sub>	1.2
GR-57-0448	Methyl salicylate	17 (3)	non-sensitizer	x			Phase I	GIVAUDAN	8834001	20001818105/AR00004728	152.15	DMSO	119-36-8	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	1.2
GR-57-0357	Isopropanol	NC (> 50%)	non-sensitizer	x			Phase II	FLUKA	59300	60450	60.10	DMSO	67-63-0	C <sub>3</sub> H <sub>8</sub> O	0.4
GR-60-5996	Chlorobenzene	Neg. (4)	non-sensitizer	x			Phase I	FLUKA	8650	1389822 44708183	112.56	DMSO	108-90-7	C <sub>6</sub> H <sub>5</sub> Cl	2.4
GR-60-8090	Sulfanilamide	NC	non-sensitizer	x			Phase I	Riedel	46874	3097X	172.20	DMSO	63-74-1	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	-0.1
Added From SENS-it-iv List															
GR-57-0208	Diethyl phthalate	>100	non-sensitizer			x	Phase II	ALDRICH	524972	13901BJ	222.24	DMSO	84-66-2	C <sub>12</sub> H <sub>14</sub> O <sub>4</sub>	2

(1) Geometric mean 12.2 in ICCVAM database, but negative in some tests, considered negative in performance standards

(2) Negative reference according D. Basketter, 1999, Food Chem. Toxicol. 37, 1167-1174.

(3) geometric mean 17, but negative in three tests, > 20% in AOO study, considered negative in performance standards

(4) Negative reference according D. Basketter, 1999, Food Chem. Toxicol. 37, 1167-1174.