

Attachment 9_Chemicals used to assess between laboratory reproducibility

Givaudan-ID	Name	EC3, Geo Mean ICCVAM database	Classification	Blind Code	Source	Order Number	Batch Number	MW	Solvent	CAS-Nr	Formula	cLogP
From list published by Casati et al., ATLA, 2009												
GR-87-1787	Oxazolone	0.0028	strong-extreme	BC_07	SIGMA	E0753	124K3690	217.22	DMSO	15646-46-5	C ₁₂ H ₁₁ NO ₃	1.9
GR-87-1790	4-Phenylenediamine	0.11	strong-extreme	BC_01	ALDRICH	78429	1416291 41609223	108.14	DMSO	106-50-3	C ₆ H ₈ N ₂	0.9
GR-82-2963	Cinnamic aldehyde	1.3	moderate	BC_02	GIVAUDAN	1500001	9000538811	132.16	DMSO	104-55-2	C ₉ H ₈ O	1.9
GR-01-1375	Isoeugenol	1.5	moderate	BC_05	GIVAUDAN	6237001	9000691084	164.20	DMSO	97-54-1	C ₁₀ H ₁₂ O ₂	2.4
GR-60-8400	tetramethylthiuramdisulfide	3.1	moderate	BC_20	FLUKA	87940	374481/1 12307426	296.54	DMSO	137-26-8	C ₁₀ H ₂₀ N ₂ S ₄	2.7
GR-60-7976	2-Mercaptobenzothiazole	2.5	moderate	BC_08	FLUKA	63720	014801/1 42506102	167.25	DMSO	149-30-4	C ₇ H ₅ NS ₂	2.4
GR-57-0251	Eugenol	10.1	weak	BC_06	GIVAUDAN	5002001	9000724417	164.20	DMSO	97-53-0	C ₁₀ H ₁₂ O ₂	2.1
GR-57-0143	Cinnamyl alcohol	21.0	weak	BC_18	GIVAUDAN	1173001	9000626366	134.18	DMSO	104-54-1	C ₉ H ₁₀ O	1.7
GR-60-3682	Glyoxal	0.7	strong-extreme	BC_14	SIGMA	128465	1414774 50909111	58.04	DMSO	107-22-2	C ₂ H ₂ O ₂	-0.6
GR-61-0358	4-nitrobenzylbromide	0.05	strong-extreme	BC_03	FLUKA	73170	249839 686	216.03	DMSO	100-11-8	C ₇ H ₆ BrNO ₂	2.8
GR-87-1796	Methyldibromo glutaronitrile	0.9 /1.9	moderate	BC_13	FLUKA	34392	1386163 12009244	265.93	DMSO	35691-65-7	C ₆ H ₆ Br ₂ N ₂	2.3
GR-60-4237	Salicylic acid	12.2 (1)	non-sensitizer	BC_11	FLUKA	84210	puriss	138.12	DMSO	69-72-7	C ₇ H ₆ O ₃	1.1
GR-60-0595	Sodium lauryl sulfate	false positive	non-sensitizer	BC_10	FLUKA	71727	371996/1 51998	288.38	DMSO	151-21-3	C ₁₂ H ₂₅ NaO ₄ S	3.4
GR-60-2116	Lactic acid	Neg. (2)	non-sensitizer	BC_19	FLUKA	69775	1433079 41209P09	90.08	DMSO	50-21-5	C ₃ H ₆ O ₃	-0.5
GR-60-0500	Glycerol	NC (> 100%)	non-sensitizer	BC_15	FLUKA	49780	364809/1 54097	92.09	DMSO	56-81-5	C ₃ H ₈ O ₃	-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	BC_04	FLUKA	69749	1413786 20809206	221.23	H2O / 100 mM	55-55-0	C ₇ H ₁₁ NO ₅ S	1.4
GR-87-1788	(5-chloro)-Methylisothiazolinone	0.01	strong-extreme	BC_09	FLUKA	00344	1292199 54406084	149.60	H2O /50 mM	2682-20-4	C ₄ H ₄ ClNOS	1.2
GR-60-2407	Phenyl benzoate	13.6	weak	BC_21	ALDRICH	14,271-9	09157-508	198.22	DMSO	93-99-2	C ₁₃ H ₁₀ O ₂	2.9
GR-87-1799	Imidazolidinyl urea	24.0	weak	BC_12	SIGMA	I5133	048K0664	388.29	DMSO	39236-46-9	C ₁₁ H ₁₆ N ₈ O ₈	-4.8
GR-57-0357	Isopropanol	NC (> 50%)	non-sensitizer	BC_17	FLUKA	59300	60450	60.10	DMSO	67-63-0	C ₃ H ₈ O	0.4
Added From SENS-it-iv List												
GR-57-0208	Diethyl phthalate	>100	non-sensitizer	BC_16	ALDRICH	524972	13901BJ	222.24	DMSO	84-66-2	C ₁₂ H ₁₄ O ₄	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.