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**Appendix C**

**Comparative LLNA: DA, Traditional LLNA, Guinea Pig, and Human Skin  
Sensitization Data**

**C1 Comparison of LLNA: DA, Traditional LLNA, Guinea Pig, and Human Results  
(Alphanumeric Order).....C-3**

**C2 Comparison of Alternative LLNA: DA Decision Criteria and Traditional  
LLNA Results (Alphanumeric Order).....C-15**

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## **Appendix C1**

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### **Comparison of LLNA: DA, Traditional LLNA, Guinea Pig, and Human Results**

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**(Alphanumeric Order)**

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48 **Appendix C-1 Comparative Performance of the LLNA: DA, Traditional LLNA, Guinea Pig, and Human Tests**  
 49 **(Alphanumeric Order)**

Substance Name	CASRN	LLNA: DA Highest Conc. Tested (%)	LLNA: DA Highest SI <sup>1</sup>	LLNA: DA Reference	Trad. LLNA Result	GP Result <sup>2</sup>	Human Result <sup>3</sup>	Trad. LLNA Reference	GP Reference	Human Reference	Skin Irritant?	Skin Irritation Data Reference
Abietic acid	514-10-3	25	6.26	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	No at ≤ 2.5% (GP)	Basketter et al. 2007
Abietic acid	514-10-3	25	4.64	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	No at ≤ 2.5% (GP)	Basketter et al. 2007
Abietic acid	514-10-3	25	7.96	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	No at ≤ 2.5% (GP)	Basketter et al. 2007
Abietic acid	514-10-3	25	3.98 at 10%	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	No at ≤ 2.5% (GP)	Basketter et al. 2007
3-Aminophenol	591-27-5	10	2.83	Omori et al. 2008	+	NA	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 5% (GP)	Basketter et al. 2007b
3-Aminophenol	591-27-5	10	1.76 at 3%	Omori et al. 2008	+	NA	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 5% (GP)	Basketter et al. 2007b
3-Aminophenol	591-27-5	10	2.38	Omori et al. 2008	+	NA	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 5% (GP)	Basketter et al. 2007b
Benzalkonium chloride	8001-54-5	2.5	6.68	Idehara et al. 2008	+	-	+	Gerberick 1992	ICCVAM 1999	ICCVAM 1999	Irritant at 2% ACE (mice)	Gerberick et al 2002 Manetz et al. 1999
Benzocaine	94-09-7	25	4.84	Idehara et al. 2008	+/- <sup>4</sup>	+	+/-	ICCVAM 1999	ICCVAM 1999	Poole et al. 1970; ICCVAM 1999 (Equivocal data)	Negative at ≤ 10% (GP)	Basketter and Scholes
p-Benzoquinone	106-51-4	0.100	3.79	Idehara unpublished	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Nonirritant at 2.5% (GP)	Basketter et al. 2007b
1-Bromobutane	109-65-9	25	1.65	Idehara et al. 2008	-	NA	NA	ICCVAM 1999	NA	NA	NA	NA
Butyl glycidyl ether	2426-08-6	50	4.59	Idehara unpublished	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 0.1% (GP)	Wahlberg and Boman 1985
Chlorobenzene	108-90-7	25	2.44	Idehara et al. 2008	-	-	NA	ICCVAM 1999	ICCVAM 1999	NA	No data. Low irritancy	Basketter et al. 1998

Substance Name	CASRN	LLNA: DA Highest Conc. Tested (%)	LLNA: DA Highest SI <sup>1</sup>	LLNA: DA Reference	Trad. LLNA Result	GP Result <sup>2</sup>	Human Result <sup>3</sup>	Trad. LLNA Reference	GP Reference	Human Reference	Skin Irritant?	Skin Irritation Data Reference
											potential assumed based on clinical literature.	
5-Chloro-2-methyl-4-isothiazolin-3-one	26172-55-4	0.100	7.50	Idehara unpublished	+	+	+	ICCVAM 1999; Gerberick et al. 2005	ICCVAM 1999	ICCVAM 1999	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
Cinnamic alcohol	104-54-1	90	5.66 at 50%	Idehara unpublished	+	+	+	Gerberick et al. 2005	Robinson et al. 1990	Jordan and King 1977	Nonirritant at 1% (GP)	Robinson et al. 1990
Cinnamic aldehyde	104-55-2	15	4.73	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 0.75% (GP); Mild Irritant at 100% (rabbits)	Basketter et al. 2007b; ECETOC #66, 1995
Citral	5392-40-5	25	4.40	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 0.5% (GP)	Basketter et al. 2007b
Cobalt chloride	7646-79-9	5	3.64	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Negative at ≤ 0.5% (GP)	Basketter and Scholes
Cobalt chloride	7646-79-9	1 <sup>5</sup>	2.66	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Negative at ≤ 0.5% (GP)	Basketter and Scholes
Cobalt chloride	7646-79-9	3	20.55	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Negative at ≤ 0.5% (GP)	Basketter and Scholes
Cobalt chloride	7646-79-9	3	8.07	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Negative at ≤ 0.5% (GP)	Basketter and Scholes
Cobalt chloride	7646-79-9	5	2.01	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Negative at ≤ 0.5% (GP)	Basketter and Scholes
Cobalt chloride	7646-79-9	5	2.54	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Negative at ≤ 0.5% (GP)	Basketter and Scholes
Cobalt chloride	7646-79-9	5	4.25	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Negative at ≤ 0.5% (GP)	Basketter and Scholes
Cobalt chloride	7646-79-9	5	5.06	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Negative at ≤ 0.5% (GP)	Basketter and Scholes

Substance Name	CASRN	LLNA: DA Highest Conc. Tested (%)	LLNA: DA Highest SI <sup>1</sup>	LLNA: DA Reference	Trad. LLNA Result	GP Result <sup>2</sup>	Human Result <sup>3</sup>	Trad. LLNA Reference	GP Reference	Human Reference	Skin Irritant?	Skin Irritation Data Reference
Diethyl maleate	141-05-9	10.0	3.78	Idehara unpublished				Gerberick et al. 2005	NA	Marzulli and Maibach 1980	Nonirritant at 100% (GP)	Basketter et al. 2007b
Diethyl phthalate	84-66-2	100	1.09	Idehara et al. 2008	-	-	-	Gerberick et al. 2005	Klecak et al. 1977	Schneider and Akkan 2004	Negative at 100% (rabbits)	ECETOC #66, 1995
Dimethyl isophthalate	1459-93-4	25	0.89 at 5%	Idehara unpublished	-	-	-	ICCVAM 1999; Basketter et al. 1999b	ICCVAM 1999; Basketter et al. 1999b	Basketter et al. 1999b	Negative at ≤ 10% (GP)	Basketter and Scholes
Dimethyl isophthalate	1459-93-4	25	1.34 at 5%	Omori et al. 2008	-	-	-	ICCVAM 1999; Basketter et al. 1999b	ICCVAM 1999; Basketter et al. 1999b	Basketter et al. 1999b	Negative at ≤ 10% (GP)	Basketter and Scholes
Dimethyl isophthalate	1459-93-4	25	1.00 at 5%	Omori et al. 2008	-	-	-	ICCVAM 1999; Basketter et al. 1999b	ICCVAM 1999; Basketter et al. 1999b	Basketter et al. 1999b	Negative at ≤ 10% (GP)	Basketter and Scholes
Dimethyl isophthalate	1459-93-4	25	1.26 at 5%	Omori et al. 2008	-	-	-	ICCVAM 1999; Basketter et al. 1999b	ICCVAM 1999; Basketter et al. 1999b	Basketter et al. 1999b	Negative at ≤ 10% (GP)	Basketter and Scholes
2,4-Dinitrochlorobenzene	97-00-7	1	7.10	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
2,4-Dinitrochlorobenzene	97-00-7	0.30	11.97	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
2,4-Dinitrochlorobenzene	97-00-7	0.30	9.23	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
2,4-Dinitrochlorobenzene	97-00-7	0.30	9.96	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
2,4-Dinitrochlorobenzene	97-00-7	0.30	8.53	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b

Substance Name	CASRN	LLNA: DA Highest Conc. Tested (%)	LLNA: DA Highest SI <sup>1</sup>	LLNA: DA Reference	Trad. LLNA Result	GP Result <sup>2</sup>	Human Result <sup>3</sup>	Trad. LLNA Reference	GP Reference	Human Reference	Skin Irritant?	Skin Irritation Data Reference
2,4-Dinitrochlorobenzene	97-00-7	0.30	7.86	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
2,4-Dinitrochlorobenzene	97-00-7	0.30	15.14	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
2,4-Dinitrochlorobenzene	97-00-7	0.30	13.18	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
2,4-Dinitrochlorobenzene	97-00-7	0.30	12.60	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
2,4-Dinitrochlorobenzene	97-00-7	0.30	10.89	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
2,4-Dinitrochlorobenzene	97-00-7	0.30	4.71	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
2,4-Dinitrochlorobenzene	97-00-7	1	7.10	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Schneider and Akkan 2004	Nonirritant at 0.1% (GP)	Basketter et al. 2007b
Ethyl acrylate	140-88-5	50	4.29 at 25%	Idehara unpublished	+	-	+	Gerberick et al. 2005	Van der Walle et al. 1982	Marzulli and Maibach 1974	Nonirritant at 0.3 M (GP)	Van der Walle et al. 1982
Ethylene glycol dimethacrylate	97-90-5	50	4.45	Idehara unpublished	+	-	+	ICCVAM 1999	ICCVAM 1999; Gerberick 1992	ICCVAM 1999; Basketter et al. 1999b	Nonirritant at 1% (GP)	Wahlberg and Boman 1985
Eugenol	97-53-0	25	7.07	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 25% (GP); Mild irritant at 100% (rabbits)	Basketter et al. 2007b; ECETOC #66, 1995
Formaldehyde	50-00-0	2.50	5.10	Idehara et al. 2008	+	+	+	Gerberick et al. 2005;	ICCVAM 1999	ICCVAM 1999; Kwon et	Nonirritant at 2% (GP)	Basketter et al.

Substance Name	CASRN	LLNA: DA Highest Conc. Tested (%)	LLNA: DA Highest SI <sup>1</sup>	LLNA: DA Reference	Trad. LLNA Result	GP Result <sup>2</sup>	Human Result <sup>3</sup>	Trad. LLNA Reference	GP Reference	Human Reference	Skin Irritant?	Skin Irritation Data Reference
								Hilton et al. 1998		al. 2003		2007b
Formaldehyde	50-00-0	5.0	4.84	Omori et al. 2008	+	+	+	Gerberick et al. 2005; Hilton et al. 1998	ICCVAM 1999	ICCVAM 1999; Kwon et al. 2003	Nonirritant at 2% (GP)	Basketter et al. 2007b
Formaldehyde	50-00-0	5.0	3.18	Omori et al. 2008	+	+	+	Gerberick et al. 2005; Hilton et al. 1998	ICCVAM 1999	ICCVAM 1999; Kwon et al. 2003	Nonirritant at 2% (GP)	Basketter et al. 2007b
Formaldehyde	50-00-0	5.0	2.69	Omori et al. 2008	+	+	+	Gerberick et al. 2005; Hilton et al. 1998	ICCVAM 1999	ICCVAM 1999; Kwon et al. 2003	Nonirritant at 2% (GP)	Basketter et al. 2007b
Glutaraldehyde	111-30-8	0.25	6.45	Idehara et al. 2008	+	+	+	Basketter et al. 2005; Hilton et al. 1998	Gad et al. 1986	Marzulli et al. 1974; Schneider and Akkan 2004	NA	NA
Glutaraldehyde	111-30-8	0.50	5.00	Omori et al. 2008	+	+	+	Basketter et al. 2005; Hilton et al. 1998	Gad et al. 1986	Marzulli et al. 1974; Schneider and Akkan 2004	NA	NA
Glutaraldehyde	111-30-8	0.50	3.39	Omori et al. 2008	+	+	+	Basketter et al. 2005; Hilton et al. 1998	Gad et al. 1986	Marzulli et al. 1974; Schneider and Akkan 2004	NA	NA
Glutaraldehyde	111-30-8	0.50	2.57	Omori et al. 2008	+	+	+	Basketter et al. 2005; Hilton et al. 1998	Gad et al. 1986	Marzulli et al. 1974; Schneider and Akkan 2004	NA	NA
Hexane	110-54-3	100	2.31	Idehara et al. 2008	-	NA	-	ICCVAM 1999	NA	ICCVAM 1999	Irritant at 100% (humans)	Kligman 1966c
Hexyl cinnamic aldehyde	101-86-0	25	6.47	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	5.78	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	4.82	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	4.44	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995



Substance Name	CASRN	LLNA: DA Highest Conc. Tested (%)	LLNA: DA Highest SI <sup>1</sup>	LLNA: DA Reference	Trad. LLNA Result	GP Result <sup>2</sup>	Human Result <sup>3</sup>	Trad. LLNA Reference	GP Reference	Human Reference	Skin Irritant?	Skin Irritation Data Reference
Hexyl cinnamic aldehyde	101-86-0	25	5.11	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	3.97	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	5.50	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	7.09	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	10.22	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	3.88	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	3.51	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	4.47	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	5.71	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	5.41	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	7.60	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	3.92	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	8.42	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hexyl cinnamic aldehyde	101-86-0	25	6.45	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Mild irritant at 100% (rabbits)	ECETOC #66, 1995
Hydroxycitronellal	107-75-5	50	5.69	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 50% (GP); Negative at 100% (rabbits)	Basketter et al. 2007b; ECETOC #66, 1995
Imidazolidinyl urea	39236-46-9	50	4.67	Idehara et al. 2008	+	+	+	Gerberick et al. 2005	ICCVAM 1999	ICCVAM 1999	Negative at ≤ 75% (GP)	Basketter and Scholes
Isoeugenol	97-54-1	50	12.36 at 25%	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 5% (GP)	Basketter et al. 2007b
Isoeugenol	97-54-1	10	6.11	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 5% (GP)	Basketter et al.

Substance Name	CASRN	LLNA: DA Highest Conc. Tested (%)	LLNA: DA Highest SI <sup>1</sup>	LLNA: DA Reference	Trad. LLNA Result	GP Result <sup>2</sup>	Human Result <sup>3</sup>	Trad. LLNA Reference	GP Reference	Human Reference	Skin Irritant?	Skin Irritation Data Reference
												2007b
Isoeugenol	97-54-1	10	5.54	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 5% (GP)	Basketter et al. 2007b
Isoeugenol	97-54-1	10	7.09	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 5% (GP)	Basketter et al. 2007b
Isopropanol	67-63-0	50	1.08 at 25%	Idehara et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Isopropanol	67-63-0	50	1.54 at 10%	Omori et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Isopropanol	67-63-0	50	0.91 at 10%	Omori et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Isopropanol	67-63-0	50	1.01 at 10%	Omori et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Isopropanol	67-63-0	50	1.57 at 10%	Omori et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Isopropanol	67-63-0	50	0.76 at 25%	Omori et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Isopropanol	67-63-0	50	1.97 at 10%	Omori et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Isopropanol	67-63-0	50	1.45 at 10%	Omori et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Isopropanol	67-63-0	50	1.21 at 10%	Omori et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Isopropanol	67-63-0	50	0.70 at 25%	Omori et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Isopropanol	67-63-0	50	1.25	Omori et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	Kwon et al. 2003	Negative at 100% (rabbits)	ECETOC #66, 1995
Lactic acid	50-21-5	50	1.06 at 10%	Idehara et al. 2008	-	-	-	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Slightly irritating at 10% aq. (rabbits)	Cosmetic Ingredient Review Expert Panel 1998
Lactic acid	50-21-5	25	0.93 at 5%	Omori et al. 2008	-	-	-	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Slightly irritating at 10% aq. (rabbits)	Cosmetic Ingredient Review Expert Panel

Substance Name	CASRN	LLNA: DA Highest Conc. Tested (%)	LLNA: DA Highest SI <sup>1</sup>	LLNA: DA Reference	Trad. LLNA Result	GP Result <sup>2</sup>	Human Result <sup>3</sup>	Trad. LLNA Reference	GP Reference	Human Reference	Skin Irritant?	Skin Irritation Data Reference
												1998
Lactic acid	50-21-5	25	0.99 at 5%	Omori et al. 2008	-	-	-	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Slightly irritating at 10% aq. (rabbits)	Cosmetic Ingredient Review Expert Panel 1998
Lactic acid	50-21-5	25	0.97 at 10%	Omori et al. 2008	-	-	-	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Slightly irritating at 10% aq. (rabbits)	Cosmetic Ingredient Review Expert Panel 1998
Lactic acid	50-21-5	25	0.91	Omori et al. 2008	-	-	-	ICCVAM 1999	ICCVAM 1999	Basketter et al. 1999b	Slightly irritating at 10% aq. (rabbits)	Cosmetic Ingredient Review Expert Panel 1998
2-Mercaptobenzo-thiazole	149-30-4	50	2.00	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 10% (GP)	Basketter et al. 2007b
Methyl methacrylate	80-62-6	100	1.81	Idehara unpublished	+	+	+ (case studies, no exposure concentration)	Betts et al. 2006	Van der Walle et al. 1982	Betts et al. 2006	Nonirritant at 3 M (GP)	Van der Walle et al. 1982
Methyl salicylate	119-36-8	25	1.20	Idehara et al. 2008	-	-	-	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Irritant at 10% AOO (mice)	Gerberick et al 2002
Methyl salicylate	119-36-8	25	1.55	Omori et al. 2008	-	-	-	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Irritant at 10% AOO (mice)	Gerberick et al 2002
Methyl salicylate	119-36-8	25	1.77 at 10%	Omori et al. 2008	-	-	-	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Irritant at 10% AOO (mice)	Gerberick et al 2002
Methyl salicylate	119-36-8	25	0.83	Idehara et al. 2008	-	-	-	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Irritant at 10% AOO (mice)	Gerberick et al 2002
Nickel (II) chloride	7718-54-9	10	1.30	Idehara unpublished	-	+	+	ICCVAM 1999	ICCVAM 1999	Vandenbergh and Epstein 1963	Negative at ≤ 0.15% (GP)	Basketter and Scholes
Nickel (II) sulfate hexahydrate	10101-97-0	5.0	2.17 at 2.5%	Omori et al. 2008	+	+	+	Ryan et al. 2002	ICCVAM 1999	ICCVAM 1999	Irritant at 10% (humans);	Kligman 1966c;

Substance Name	CASRN	LLNA: DA Highest Conc. Tested (%)	LLNA: DA Highest SI <sup>1</sup>	LLNA: DA Reference	Trad. LLNA Result	GP Result <sup>2</sup>	Human Result <sup>3</sup>	Trad. LLNA Reference	GP Reference	Human Reference	Skin Irritant?	Skin Irritation Data Reference
											Nonirritant at 0.15% (GP)	Scholes et al. 1992
Nickel (II) sulfate hexahydrate	10101-97-0	10	1.52 at 3%	Omori et al. 2008	+	+	+	Ryan et al. 2002	ICCVAM 1999	ICCVAM 1999	Irritant at 10% (humans); Nonirritant at 0.15% (GP)	Kligman 1966c; Scholes et al. 1992
Nickel (II) sulfate hexahydrate	10101-97-0	10	11.78	Omori et al. 2008	+	+	+	Ryan et al. 2002	ICCVAM 1999	ICCVAM 1999	Irritant at 10% (humans); Nonirritant at 0.15% (GP)	Kligman 1966c; Scholes et al. 1992
Nickel (II) sulfate hexahydrate	10101-97-0	10	3.49 at 1%	Omori et al. 2008	+	+	+	Ryan et al. 2002	ICCVAM 1999	ICCVAM 1999	Irritant at 10% (humans); Nonirritant at 0.15% (GP)	Kligman 1966c; Scholes et al. 1992
Nickel (II) sulfate hexahydrate	10101-97-0	10	0.79 at 3%	Omori et al. 2008	+	+	+	Ryan et al. 2002	ICCVAM 1999	ICCVAM 1999	Irritant at 10% (humans); Nonirritant at 0.15% (GP)	Kligman 1966c; Scholes et al. 1992
Nickel (II) sulfate hexahydrate	10101-97-0	10	1.24 at 3%	Omori et al. 2008	+	+	+	Ryan et al. 2002	ICCVAM 1999	ICCVAM 1999	Irritant at 10% (humans); Nonirritant at 0.15% (GP)	Kligman 1966c; Scholes et al. 1992
Nickel (II) sulfate hexahydrate	10101-97-0	10	2.13	Omori et al. 2008	+	+	+	Ryan et al. 2002	ICCVAM 1999	ICCVAM 1999	Irritant at 10% (humans); Nonirritant at 0.15% (GP)	Kligman 1966c; Scholes et al. 1992
Nickel (II) sulfate hexahydrate	10101-97-0	10	1.56 at 3%	Omori et al. 2008	+	+	+	Ryan et al. 2002	ICCVAM 1999	ICCVAM 1999	Irritant at 10% (humans); Nonirritant at 0.15% (GP)	Kligman 1966c; Scholes et al. 1992
Phenyl benzoate	93-99-2	10	4.24 at 5%	Idehara unpublished	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al 2005a	NA	NA
p-Phenylenediamine	106-50-3	1	5.14 at 0.25%	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 0.5% (GP)	Basketter et al. 2007b
Phthalic anhydride	85-44-9	1.0	5.49	Idehara et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	Basketter et al. 2001	Negative at ≤ 10% (GP)	Basketter and Scholes
Potassium dichromate	7778-50-9	1.0	4.78	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 0.15% (GP)	Basketter et al. 2007b

Substance Name	CASRN	LLNA: DA Highest Conc. Tested (%)	LLNA: DA Highest SI <sup>1</sup>	LLNA: DA Reference	Trad. LLNA Result	GP Result <sup>2</sup>	Human Result <sup>3</sup>	Trad. LLNA Reference	GP Reference	Human Reference	Skin Irritant?	Skin Irritation Data Reference
Potassium dichromate	7778-50-9	1.0	4.08	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 0.15% (GP)	Basketter et al. 2007b
Potassium dichromate	7778-50-9	1.0	6.01	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 0.15% (GP)	Basketter et al. 2007b
Potassium dichromate	7778-50-9	1.0	6.37	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 0.15% (GP)	Basketter et al. 2007b
Potassium dichromate	7778-50-9	1.0	5.49	Omori et al. 2008	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 0.15% (GP)	Basketter et al. 2007b
Propyl gallate	121-79-9	2.5	4.95	Idehara unpublished	+	+	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 5% (GP)	Basketter and Scholes
Propylparaben	94-13-3	25	1.28	Idehara et al. 2008	-	-	+	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Nonirritant at 10% (GP)	Basketter and Scholes
Resorcinol	108-46-3	25	4.33	Idehara et al. 2008	+	-	+	Basketter et al. 2007	ICCVAM 1999	ICCVAM 1999; Basketter et al. 2007	Nonirritant at 15% (humans)	Kligman 1966c
Salicylic acid	69-72-7	25	2.00	Idehara unpublished	-	-	+(6/23 at 1%)	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999 (Kligman 1966b for nickel sulfate)	Irritant at 20% aq. (mice)	Gerberick et al. 2002
Sodium lauryl sulfate	151-21-3	10	3.39	Idehara et al. 2008	+	-	-	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999	Irritant at 20% (rabbits)	ECETOC #66, 1995
Sulfanilamide	63-74-1	50	0.86 at 25%	Idehara unpublished	-	-	-	ICCVAM 1999	ICCVAM 1999	ICCVAM 1999; Kligman 1966c	Nonirritant at 25% (humans)	Kligman 1966c
Toluene 2,4-diisocyanate	584-84-9	0.25	9.43	Idehara et al. 2008	+	+	+	van Och et al. 2001	NA	Basketter et al. 2001	NA	NA
Trimellitic anhydride	552-30-7	0.50	4.96	Idehara et al. 2008	+	+	NA	ICCVAM 1999; Basketter and Scholes 1992	ICCVAM 1999; Gad et al. 1986	ICCVAM 1999; Basketter et al. 2001	Negative at ≤ 10% (GP)	Basketter and Scholes

Abbreviations: ACE = acetone; AOO = acetone: olive oil (4:1); aq. = aqueous; CASRN = Chemical Abstracts Service Registry Number; Conc. = concentration; ECETOC = European Centre for Ecotoxicology and Toxicology of Chemicals; GP = guinea pig; LLNA = murine local lymph node assay; LLNA: DA = murine local lymph node assay modified by Daicel Chemical Industries, Ltd. based on ATP content; NA = not available; SI = stimulation index; Trad. = traditional;

“+” = Sensitizer.

“-” = Nonsensitizer.

- 55 <sup>1</sup>Highest SI achieved at highest concentration tested, unless otherwise noted.  
56 <sup>2</sup>GP refers to outcomes obtained by studies conducted using either the guinea pig maximization test or the Buehler test.  
57 <sup>3</sup>Human refers to outcomes obtained by studies conducted using the human maximization test, inclusion of the test substance in a human patch test allergen kit, and/or published clinical case  
58 studies/reports.  
59 <sup>4</sup>Equivocal traditional LLNA data (ICCVAM 1999); substance not included in accuracy analyses.  
60 <sup>5</sup>Data not reported for the highest dose (i.e., 3%), only for 0.3% and 1%.  
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## **Appendix C2**

76 **Comparison of Alternative LLNA: DA Decision Criteria and Traditional LLNA Results**

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**(Alphanumeric Order)**

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92 **Appendix C-2 Comparative Performance of Various LLNA: DA SI Values and Traditional LLNA Tests (Alphanumeric**  
 93 **Order)**

Substance Name	CASRN	Highest Conc. Tested (%)	Highest SI <sup>1</sup>	≥95% CI	≥3 SD	≥2 SD	Stats. <sup>2</sup>	SI ≥ 5.0	SI ≥ 4.5	SI ≥ 4.0	SI ≥ 3.5	SI ≥ 3.0	SI ≥ 2.5	SI ≥ 2.0	SI ≥ 1.5	SI ≥ 1.3	SI ≥ 1.0	LLNA: DA Ref.	Trad. LLNA Result	Trad. LLNA Ref.
Abietic acid	514-10-3	25	6.26	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Abietic acid	514-10-3	25	4.64	+	+	+	+	-	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Abietic acid	514-10-3	25	7.96	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Abietic acid	514-10-3	25	3.98 at 10%	+	+	+	+	-	-	-	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
3-Aminophenol	591-27-5	10	2.83	+	+	+	+	-	-	-	-	-	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
3-Aminophenol	591-27-5	10	1.76 at 3%	+	+	+	+	-	-	-	-	-	-	-	+	+	+	Omori et al. 2008	+	ICCVAM 1999
3-Aminophenol	591-27-5	10	2.38	+	+	+	+	-	-	-	-	-	-	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Benzalkonium chloride	8001-54-5	2.5	6.68	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	Gerberick 1992
Benzocaine	94-09-7	25	4.84	+	+	+	+	-	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+/- <sup>3</sup>	ICCVAM 1999
p-Benzoquinone	106-51-4	0.100	3.79	+	+	+	+	-	-	-	+	+	+	+	+	+	+	Idehara unpublished	+	ICCVAM 1999
1-Bromobutane	109-65-9	25	1.65	+	+	+	+	-	-	-	-	-	-	-	+	+	+	Idehara et al. 2008	-	ICCVAM 1999
Butyl glycidyl ether	2426-08-6	50	4.59	+	-	+	+	-	+	+	+	+	+	+	+	+	+	Idehara unpublished	+	ICCVAM 1999
Chlorobenzene	108-90-7	25	2.44	+	+	+	+	-	-	-	-	-	-	+	+	+	+	Idehara et al. 2008	-	ICCVAM 1999

Substance Name	CASRN	Highest Conc. Tested (%)	Highest SI <sup>1</sup>	≥95 % CI	≥3 SD	≥2 SD	Stats. <sup>2</sup>	SI ≥ 5.0	SI ≥ 4.5	SI ≥ 4.0	SI ≥ 3.5	SI ≥ 3.0	SI ≥ 2.5	SI ≥ 2.0	SI ≥ 1.5	SI ≥ 1.3	SI ≥ 1.0	LLNA: DA Ref.	Trad. LLNA Result	Trad. LLNA Ref.
5-Chloro-2-methyl-4-isothiazolin-3-one	26172-55-4	0.100	7.50	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara unpublished	+	ICCVAM 1999; Gerberick et al. 2005
Cinnamic alcohol	104-54-1	90	5.66 at 50%	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara unpublished	+	Gerberick et al. 2005
Cinnamic aldehyde	104-55-2	15	4.73	+	+	+	+	-	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Citral	5392-40-5	25	4.40	+	+	+	+	-	-	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Cobalt chloride	7646-79-9	5	3.64	+	+	+	+	-	-	-	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Cobalt chloride	7646-79-9	1 <sup>4</sup>	2.66	+	+	+	+	-	-	-	-	-	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Cobalt chloride	7646-79-9	3	20.55	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Cobalt chloride	7646-79-9	3	8.07	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Cobalt chloride	7646-79-9	5	2.01	+	+	+	+	-	-	-	-	-	-	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Cobalt chloride	7646-79-9	5	2.54	+	+	+	+	-	-	-	-	-	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Cobalt chloride	7646-79-9	5	4.25	+	+	+	+	-	-	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Cobalt chloride	7646-79-9	5	5.06	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Diethyl maleate	141-05-9	10.0	3.78	+	+	+	+	-	-	-	+	+	+	+	+	+	+	Idehara unpublished	+	Gerberick et al. 2005

Substance Name	CASRN	Highest Conc. Tested (%)	Highest SI <sup>1</sup>	≥95 % CI	≥3 SD	≥2 SD	Stats. <sup>2</sup>	SI ≥ 5.0	SI ≥ 4.5	SI ≥ 4.0	SI ≥ 3.5	SI ≥ 3.0	SI ≥ 2.5	SI ≥ 2.0	SI ≥ 1.5	SI ≥ 1.3	SI ≥ 1.0	LLNA: DA Ref.	Trad. LLNA Result	Trad. LLNA Ref.
Diethyl phthalate	84-66-2	100	1.09	+	-	-	-	-	-	-	-	-	-	-	-	-	+	Idehara et al. 2008	-	Gerberick et al. 2005
Dimethyl isophthalate	1459-93-4	25	0.89 at 5%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Idehara unpublished	-	ICCVAM 1999; Basketter et al. 1999b
Dimethyl isophthalate	1459-93-4	25	1.34 at 5%	+	-	-	-	-	-	-	-	-	-	-	-	+	+	Omori et al. 2008	-	ICCVAM 1999; Basketter et al. 1999b
Dimethyl isophthalate	1459-93-4	25	1.00 at 5%	+	-	-	-	-	-	-	-	-	-	-	-	-	+	Omori et al. 2008	-	ICCVAM 1999; Basketter et al. 1999b
Dimethyl isophthalate	1459-93-4	25	1.26 at 5%	+	-	-	-	-	-	-	-	-	-	-	-	-	+	Omori et al. 2008	-	ICCVAM 1999; Basketter et al. 1999b
2,4-Dinitrochlorobenzene	97-00-7	1	7.10	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
2,4-Dinitrochlorobenzene	97-00-7	0.30	11.97	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
2,4-Dinitrochlorobenzene	97-00-7	0.30	9.23	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
2,4-Dinitrochlorobenzene	97-00-7	0.30	9.96	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
2,4-Dinitrochlorobenzene	97-00-7	0.30	8.53	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999

Substance Name	CASRN	Highest Conc. Tested (%)	Highest SI <sup>1</sup>	≥95 % CI	≥3 SD	≥2 SD	Stats. <sup>2</sup>	SI ≥ 5.0	SI ≥ 4.5	SI ≥ 4.0	SI ≥ 3.5	SI ≥ 3.0	SI ≥ 2.5	SI ≥ 2.0	SI ≥ 1.5	SI ≥ 1.3	SI ≥ 1.0	LLNA: DA Ref.	Trad. LLNA Result	Trad. LLNA Ref.
2,4-Dinitrochlorobenzene	97-00-7	0.30	7.86	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
2,4-Dinitrochlorobenzene	97-00-7	0.30	15.14	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
2,4-Dinitrochlorobenzene	97-00-7	0.30	13.18	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
2,4-Dinitrochlorobenzene	97-00-7	0.30	12.60	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
2,4-Dinitrochlorobenzene	97-00-7	0.30	10.89	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
2,4-Dinitrochlorobenzene	97-00-7	0.30	4.71	+	+	+	+	-	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
2,4-Dinitrochlorobenzene	97-00-7	1	7.10	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Ethyl acrylate	140-88-5	50	4.29 at 25%	+	-	-	+	-	-	+	+	+	+	+	+	+	+	Idehara unpublished	+	Gerberick et al. 2005
Ethylene glycol dimethacrylate	97-90-5	50	4.45	+	+	+	+	-	-	+	+	+	+	+	+	+	+	Idehara unpublished	+	ICCVAM 1999
Eugenol	97-53-0	25	7.07	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Formaldehyde	50-00-0	2.50	5.10	+	+	+	+	-	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	Gerberick et al. 2005; Hilton et al. 1998
Formaldehyde	50-00-0	5.0	4.84	+	+	+	+	-	-	-	-	+	+	+	+	+	+	Omori et al. 2008	+	Gerberick et al. 2005; Hilton et al. 1998
Formaldehyde	50-00-0	5.0	3.18	+	+	+	+	-	-	-	-	-	+	+	+	+	+	Omori et al. 2008	+	Gerberick et al. 2005; Hilton et al. 1998

Substance Name	CASRN	Highest Conc. Tested (%)	Highest SI <sup>1</sup>	≥95 % CI	≥3 SD	≥2 SD	Stats. <sup>2</sup>	SI ≥ 5.0	SI ≥ 4.5	SI ≥ 4.0	SI ≥ 3.5	SI ≥ 3.0	SI ≥ 2.5	SI ≥ 2.0	SI ≥ 1.5	SI ≥ 1.3	SI ≥ 1.0	LLNA: DA Ref.	Trad. LLNA Result	Trad. LLNA Ref.
Formaldehyde	50-00-0	5.0	2.69	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	Gerberick et al. 2005; Hilton et al. 1998
Glutaraldehyde	111-30-8	0.25	6.45	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	Basketter et al. 2005; Hilton et al. 1998
Glutaraldehyde	111-30-8	0.50	5.00	+	+	+	+	-	-	-	-	+	+	+	+	+	+	Omori et al. 2008	+	Basketter et al. 2005; Hilton et al. 1998
Glutaraldehyde	111-30-8	0.50	3.39	+	+	+	+	-	-	-	-	-	+	+	+	+	+	Omori et al. 2008	+	Basketter et al. 2005; Hilton et al. 1998
Glutaraldehyde	111-30-8	0.50	2.57	+	+	+	+	-	-	-	-	-	-	+	+	+	+	Omori et al. 2008	+	Basketter et al. 2005; Hilton et al. 1998
Hexane	110-54-3	100	2.31	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	-	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	6.47	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	5.78	+	+	+	+	-	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	4.82	+	+	+	+	-	-	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	4.44	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	5.11	+	+	+	+	-	-	-	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999

Substance Name	CASRN	Highest Conc. Tested (%)	Highest SI <sup>1</sup>	≥95 % CI	≥3 SD	≥2 SD	Stats. <sup>2</sup>	SI ≥ 5.0	SI ≥ 4.5	SI ≥ 4.0	SI ≥ 3.5	SI ≥ 3.0	SI ≥ 2.5	SI ≥ 2.0	SI ≥ 1.5	SI ≥ 1.3	SI ≥ 1.0	LLNA: DA Ref.	Trad. LLNA Result	Trad. LLNA Ref.
Hexyl cinnamic aldehyde	101-86-0	25	3.97	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	5.50	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	7.09	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	10.22	+	+	+	+	-	-	-	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	3.88	+	+	+	+	-	-	-	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	3.51	+	+	+	+	-	-	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	4.47	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	5.71	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	5.41	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	7.60	+	+	+	+	-	-	-	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	3.92	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	8.42	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hexyl cinnamic aldehyde	101-86-0	25	6.45	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Hydroxycitronella l	107-75-5	50	5.69	+	+	+	+	-	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Imidazolidinyl urea	39236-46-9	50	4.67	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	Gerberick et al. 2005

Substance Name	CASRN	Highest Conc. Tested (%)	Highest SI <sup>1</sup>	≥95 % CI	≥3 SD	≥2 SD	Stats. <sup>2</sup>	SI ≥ 5.0	SI ≥ 4.5	SI ≥ 4.0	SI ≥ 3.5	SI ≥ 3.0	SI ≥ 2.5	SI ≥ 2.0	SI ≥ 1.5	SI ≥ 1.3	SI ≥ 1.0	LLNA: DA Ref.	Trad. LLNA Result	Trad. LLNA Ref.
Isoeugenol	97-54-1	50	12.36 at 25%	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Isoeugenol	97-54-1	10	6.11	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Isoeugenol	97-54-1	10	5.54	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Isoeugenol	97-54-1	10	7.09	+	-	-	-	-	-	-	-	-	-	-	-	-	+	Omori et al. 2008	+	ICCVAM 1999
Isopropanol	67-63-0	50	1.08 at 25%	+	-	+	-	-	-	-	-	-	-	-	+	+	+	Idehara et al. 2008	-	ICCVAM 1999
Isopropanol	67-63-0	50	1.54 at 10%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Omori et al. 2008	-	ICCVAM 1999
Isopropanol	67-63-0	50	0.91 at 10%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Omori et al. 2008	-	ICCVAM 1999
Isopropanol	67-63-0	50	1.01 at 10%	+	-	+	+	-	-	-	-	-	-	-	+	+	+	Omori et al. 2008	-	ICCVAM 1999
Isopropanol	67-63-0	50	1.57 at 10%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Omori et al. 2008	-	ICCVAM 1999
Isopropanol	67-63-0	50	0.76 at 25%	+	+	+	-	-	-	-	-	-	-	-	+	+	+	Omori et al. 2008	-	ICCVAM 1999
Isopropanol	67-63-0	50	1.97 at 10%	+	-	+	-	-	-	-	-	-	-	-	-	+	+	Omori et al. 2008	-	ICCVAM 1999
Isopropanol	67-63-0	50	1.45 at 10%	+	-	-	-	-	-	-	-	-	-	-	-	-	+	Omori et al. 2008	-	ICCVAM 1999
Isopropanol	67-63-0	50	1.21 at 10%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Omori et al. 2008	-	ICCVAM 1999
Isopropanol	67-63-0	50	0.70 at 25%	+	-	+	-	-	-	-	-	-	-	-	-	-	+	Omori et al. 2008	-	ICCVAM 1999

Substance Name	CASRN	Highest Conc. Tested (%)	Highest SI <sup>1</sup>	≥95 % CI	≥3 SD	≥2 SD	Stats. <sup>2</sup>	SI ≥ 5.0	SI ≥ 4.5	SI ≥ 4.0	SI ≥ 3.5	SI ≥ 3.0	SI ≥ 2.5	SI ≥ 2.0	SI ≥ 1.5	SI ≥ 1.3	SI ≥ 1.0	LLNA: DA Ref.	Trad. LLNA Result	Trad. LLNA Ref.
Isopropanol	67-63-0	50	1.25	+	-	-	-	-	-	-	-	-	-	-	-	-	+	Omori et al. 2008	-	ICCVAM 1999
Lactic acid	50-21-5	50	1.06 at 10%	+	-	-	-	-	-	-	-	-	-	-	-	-	+	Idehara et al. 2008	-	ICCVAM 1999
Lactic acid	50-21-5	25	0.93 at 5%	+	-	-	+	-	-	-	-	-	-	-	-	-	+	Omori et al. 2008	-	ICCVAM 1999
Lactic acid	50-21-5	25	0.99 at 5%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Omori et al. 2008	-	ICCVAM 1999
Lactic acid	50-21-5	25	0.97 at 10%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Omori et al. 2008	-	ICCVAM 1999
Lactic acid	50-21-5	25	0.91	+	+	+	-	-	-	-	-	-	-	+	+	+	+	Omori et al. 2008	-	ICCVAM 1999
2-Mercaptobenzo-thiazole	149-30-4	50	2.00	+	-	+	-	-	-	-	-	-	-	-	-	-	+	Idehara et al. 2008	+	ICCVAM 1999
Methyl methacrylate	80-62-6	100	1.81	+	-	-	+	-	-	-	-	-	-	-	+	+	+	Idehara unpublished	+	Betts et al. 2006
Methyl salicylate	119-36-8	25	1.20	+	+	+	-	-	-	-	-	-	-	-	+	+	+	Idehara et al. 2008	-	ICCVAM 1999
Methyl salicylate	119-36-8	25	1.55	+	-	-	-	-	-	-	-	-	-	-	+	+	+	Omori et al. 2008	-	ICCVAM 1999
Methyl salicylate	119-36-8	25	1.77 at 10%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Omori et al. 2008	-	ICCVAM 1999
Methyl salicylate	119-36-8	25	0.83	+	+	+	+	-	-	-	-	-	-	+	+	+	+	Idehara et al. 2008	-	ICCVAM 1999
Nickel (II) chloride	7718-54-9	10	1.30	+	+	+	-	-	-	-	-	-	-	-	-	+	+	Idehara unpublished	-	ICCVAM 1999
Nickel (II) sulfate hexahydrate	10101-97-0	5.0	2.17 at 2.5%	+	-	-	-	-	-	-	-	-	-	-	+	+	+	Omori et al. 2008	+	Ryan et al. 2002
Nickel (II) sulfate hexahydrate	10101-97-0	10	1.52 at 3%	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	Ryan et al. 2002



Substance Name	CASRN	Highest Conc. Tested (%)	Highest SI <sup>1</sup>	≥95 % CI	≥3 SD	≥2 SD	Stats. <sup>2</sup>	SI ≥ 5.0	SI ≥ 4.5	SI ≥ 4.0	SI ≥ 3.5	SI ≥ 3.0	SI ≥ 2.5	SI ≥ 2.0	SI ≥ 1.5	SI ≥ 1.3	SI ≥ 1.0	LLNA: DA Ref.	Trad. LLNA Result	Trad. LLNA Ref.
Nickel (II) sulfate hexahydrate	10101-97-0	10	11.78	+	+	+	+	-	-	-	-	+	+	+	+	+	+	Omori et al. 2008	+	Ryan et al. 2002
Nickel (II) sulfate hexahydrate	10101-97-0	10	3.49 at 1%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Omori et al. 2008	+	Ryan et al. 2002
Nickel (II) sulfate hexahydrate	10101-97-0	10	0.79 at 3%	+	+	+	-	-	-	-	-	-	-	-	-	-	+	Omori et al. 2008	+	Ryan et al. 2002
Nickel (II) sulfate hexahydrate	10101-97-0	10	1.24 at 3%	+	+	+	+	-	-	-	-	-	-	+	+	+	+	Omori et al. 2008	+	Ryan et al. 2002
Nickel (II) sulfate hexahydrate	10101-97-0	10	2.13	+	-	-	-	-	-	-	-	-	-	-	+	+	+	Omori et al. 2008	+	Ryan et al. 2002
Nickel (II) sulfate hexahydrate	10101-97-0	10	1.56 at 3%	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	Ryan et al. 2002
Phenyl benzoate	93-99-2	10.0	4.24 at 5%	+	+	+	+	-	-	+	+	+	+	+	+	+	+	Idehara unpublished	+	ICCVAM 1999
p-Phenylenediamine	106-50-3	1	5.14 at 0.25%	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Phthalic anhydride	85-44-9	1.0	5.49	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Potassium dichromate	7778-50-9	1.0	4.78	+	+	+	+	-	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Potassium dichromate	7778-50-9	1.0	4.08	+	+	+	+	-	-	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Potassium dichromate	7778-50-9	1.0	6.01	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Potassium dichromate	7778-50-9	1.0	6.37	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Omori et al. 2008	+	ICCVAM 1999
Potassium dichromate	7778-50-9	1.0	5.49	+	+	+	-	-	-	-	-	-	-	-	-	-	+	Omori et al. 2008	+	ICCVAM 1999

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Propyl gallate	121-79-9	2.5	4.95	+	-	-	+	-	+	+	+	+	+	+	+	+	+	Idehara unpublished	+	ICCVAM 1999
Propylparaben	94-13-3	25	1.28	+	+	+	+	-	-	+	+	+	+	+	+	+	+	Idehara et al. 2008	-	ICCVAM 1999
Resorcinol	108-46-3	25	4.33	+	+	+	+	-	-	-	-	+	+	+	+	+	+	Idehara et al. 2008	+	Basketter et al. 2007
Salicylic acid	69-72-7	25	2.00	+	-	+	+	-	-	-	-	-	-	+	+	+	+	Idehara unpublished	-	ICCVAM 1999
Sodium lauryl sulfate	151-21-3	10	3.39	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999
Sulfanilamide	63-74-1	50	0.86 at 25%	-	-	-	+	-	-	-	-	-	-	-	-	-	-	Idehara unpublished	-	ICCVAM 1999
Toluene 2,4-diisocyanate	584-84-9	0.25	9.43	+	+	+	+	-	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	Van Och et al. 2001
Trimellitic anhydride	552-30-7	0.50	4.96	+	+	+	+	+	+	+	+	+	+	+	+	+	+	Idehara et al. 2008	+	ICCVAM 1999; Basketter and Scholes 1992

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; CI = confidence interval (mean ATP measurement of any treatment group is greater than 95% CI of mean ATP measurement for vehicle control group); Conc. = concentration; LLNA = murine local lymph node assay; LLNA: DA = murine local lymph node assay modified by Daicel Chemical Industries, Ltd. based on ATP content; Ref. = reference; SD = standard deviation (mean ATP measurement of any treatment group is greater than two or three SD for vehicle control group); SI = stimulation index; stats. = statistics (analysis of variance for multiple dose groups or *t*-test to compare one treatment group to the vehicle control group); Trad. = traditional.

“+” = Sensitizer.

“-” = Nonsensitizer.

<sup>1</sup>Highest SI achieved at highest concentration tested, unless otherwise noted.

<sup>2</sup>The ATP data were log-transformed prior to statistical analyses. For analysis of variance, significance at *p* < 0.05 was further tested by Dunnett’s test.

<sup>3</sup>Equivocal traditional LLNA data (ICCVAM 1999). Substance not included in accuracy analyses.

<sup>4</sup>Data not reported for the highest dose (i.e., 3%), only for 0.3% and 1%.