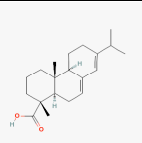
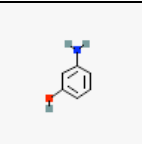
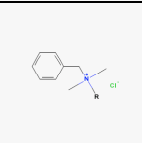
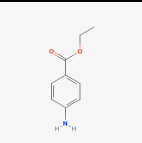
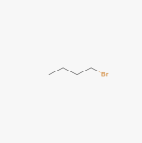
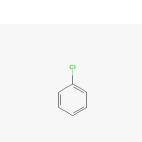
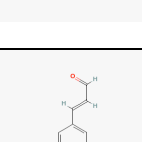


**APPENDIX B**

**Physico-Chemical Properties and Chemical Classes of Substances Tested in the  
LLNA: DA**

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


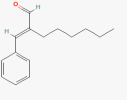
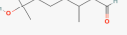
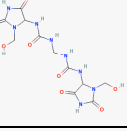

### Physico-Chemical Properties and Chemical Classes of Substances Tested in the LLNA: DA

Substance Name <sup>1</sup>	Synonyms	CASRN	Mol. Weight (g/mol)	K <sub>ow</sub> <sup>2</sup>	Peptide Reactivity <sup>3</sup>	Physical Form	Chemical Class <sup>4</sup>	Structure
Abietic acid <sup>a</sup>	Sylvic acid	514-10-3	302.46	6.46	–	Solid	Hydrocarbons, Cyclic; Polycyclic Compounds	
3-Aminophenol <sup>c</sup>	m-Aminophenol	591-27-5	109.13	0.24	–	Solid	Amines; Phenols	
Benzalkonium chloride	Alkylbenzyltrimethylammonium chloride; Germitol; Zephiral	8001-54-5	170.66	–	–	Solid/Liquid	Amines; Onium Compounds	
Benzocaine	Ethyl 4-aminobenzoate	94-09-7	165.19	1.80	–	Solid	Carboxylic Acids	
1-Bromobutane	Butyl bromide	109-65-9	137.02	2.65	Low	Liquid	Hydrocarbons, Halogenated	
Chlorobenzene	Phenyl chloride	108-90-7	112.56	2.64	Minimal	Liquid	Hydrocarbons, Cyclic; Hydrocarbons, Halogenated	
Cinnamic aldehyde	Cinnamaldehyde	104-55-2	132.16	1.82	High	Liquid	Aldehydes	







### Physico-Chemical Properties and Chemical Classes of Substances Tested in the LLNA: DA

Substance Name <sup>1</sup>	Synonyms	CASRN	Mol. Weight (g/mol)	K <sub>ow</sub> <sup>2</sup>	Peptide Reactivity <sup>3</sup>	Physical Form	Chemical Class <sup>4</sup>	Structure
Citral	2,6-Octadienal, 3,7-dimethyl-	5392-40-5	152.24	3.45	–	Liquid	Hydrocarbons, Other	
Cobalt chloride <sup>a, b</sup>	Cobaltous chloride	7646-79-9	129.84	0.85	–	Solid	Inorganic Chemical, Elements; Inorganic Chemical, Metals	
Diethyl phthalate	Ethyl phthalate	84-66-2	222.24	2.65	Minimal	Liquid	Carboxylic Acids	
Dimethyl isophthalate <sup>c</sup>	1,3-Benzenedicarboxylic acid, dimethyl ester	1459-93-4	194.19	1.66	–	Solid		
2,4-Dinitrochlorobenzene <sup>a</sup>	Dinitrochlorobenzene; DNCB	97-00-7	202.55	2.27	High	Solid	Hydrocarbons, Cyclic; Hydrocarbons, Halogenated; Nitro Compounds	
Eugenol	2-Methoxy-4-(2-propenyl)phenol; Allylguaiacol	97-53-0	164.20	2.73	–	Liquid	Carboxylic Acids	

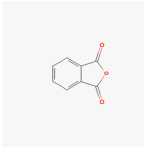

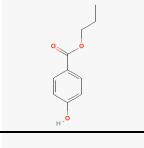
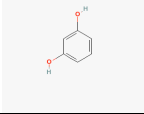
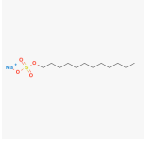
### Physico-Chemical Properties and Chemical Classes of Substances Tested in the LLNA: DA

Substance Name <sup>1</sup>	Synonyms	CASRN	Mol. Weight (g/mol)	K <sub>ow</sub> <sup>2</sup>	Peptide Reactivity <sup>3</sup>	Physical Form	Chemical Class <sup>4</sup>	Structure
Formaldehyde <sup>a</sup>	Formalin	50-00-0	30.03	0.35	Moderate	Liquid	Aldehydes	
Glutaraldehyde <sup>a</sup>	Glutaral; Pentanedial	111-30-8	100.12	-0.18	High	Liquid	Aldehydes	
Hexane	Hexyl hydride; n-Hexane	110-54-3	86.18	3.29	Minimal	Liquid	Hydrocarbons, Acyclic	
Hexyl cinnamic aldehyde <sup>a, b</sup>	alpha-Hexylcinnamaldehyde; HCA	101-86-0	216.32	4.82	Minimal	Liquid	Aldehydes	
Hydroxycitronellal	Citronellal hydrate	107-75-5	172.26	2.11	Low	Liquid	Hydrocarbons, Other	
Imidazolidinyl urea	Germall 115; Imidurea	39236-46-9	388.30	-8.28	Moderate	Solid	Urea	
Isoeugenol <sup>a</sup>	2-Methoxy-4-propenylphenol; 4-Propenylguaiacol	97-54-1	164.20	2.65	–	Liquid	Carboxylic Acids	

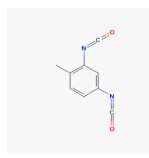
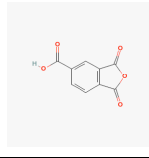
### Physico-Chemical Properties and Chemical Classes of Substances Tested in the LLNA: DA

Substance Name <sup>1</sup>	Synonyms	CASRN	Mol. Weight (g/mol)	K <sub>ow</sub> <sup>2</sup>	Peptide Reactivity <sup>3</sup>	Physical Form	Chemical Class <sup>4</sup>	Structure
Isopropanol <sup>a</sup>	Isopropyl alcohol, 2-Propanol	67-63-0	60.10	0.28	Minimal	Liquid	Alcohols	
Lactic acid <sup>b</sup>	2-Hydroxypropanoic acid	50-21-5	90.08	-0.65	Minimal	Solid	Carboxylic Acids	
2-Mercaptobenzothiazole	Captax	149-30-4	167.26	2.86	High	Solid	Heterocyclic Compounds	
Methyl salicylate <sup>a</sup>	Oil of wintergreen; Methyl 2-hydroxybenzoate	119-36-8	152.15	2.60	Minimal	Liquid	Carboxylic Acids; Phenols	
Nickel (II) sulfate hexahydrate <sup>a, b</sup>	Nickel sulfate hexahydrate	10101-97-0	154.76	—	—	Solid	Inorganic Chemical, Elements; Inorganic Chemical, Metals	
p-Phenylenediamine	4-Phenylenediamine	106-50-3	108.14	-0.39	—	Solid	Amines	

### Physico-Chemical Properties and Chemical Classes of Substances Tested in the LLNA: DA

Substance Name <sup>1</sup>	Synonyms	CASRN	Mol. Weight (g/mol)	K <sub>ow</sub> <sup>2</sup>	Peptide Reactivity <sup>3</sup>	Physical Form	Chemical Class <sup>4</sup>	Structure
Phthalic anhydride	1,2-Benzenedicarboxylic anhydride; 1,3-Dioxophthalan	85-44-9	148.12	2.07	Moderate	Solid	Anhydrides; Carboxylic Acids	
Potassium dichromate <sup>b</sup>	PDC; Dipotassium bichromate	7778-50-9	294.18	-3.59	–	Solid	Inorganic Chemical, Chromium Compounds; Inorganic Chemical, Potassium Compounds	
Propylparaben	4-Hydroxybenzoic acid, propyl ester; Propyl p-hydroxybenzoate	94-13-3	180.20	2.98	Minimal	Solid	Carboxylic Acids; Phenols	
Resorcinol	1,3-Dihydroxybenzene	108-46-3	110.11	1.03	Minimal	Solid	Phenols	
Sodium lauryl sulfate	Sodium dodecyl sulfate, SLS, SDS, Irium	151-21-3	288.38	1.69	–	Solid	Alcohols; Sulfur Compounds; Lipids	

### Physico-Chemical Properties and Chemical Classes of Substances Tested in the LLNA: DA

Substance Name <sup>1</sup>	Synonyms	CASRN	Mol. Weight (g/mol)	K <sub>ow</sub> <sup>2</sup>	Peptide Reactivity <sup>3</sup>	Physical Form	Chemical Class <sup>4</sup>	Structure
Toluene 2,4-diisocyanate	2,4-TDI	584-54-9	174.16	3.74	–	Liquid	Hydrocarbons, Cyclic; Isocyanates	
Trimellitic anhydride	4-Carboxyphthalic anhydride	552-30-7	192.13	1.95	Low	Solid	Anhydride; Carboxylic Acids	

Abbreviations: CASRN=Chemical Abstracts Registry Number; g/mol=grams per mole; Mol.=Molecular; LLNA: DA=Local Lymph Node Assay Modified by Daicel Chemical Industries, Ltd. Based on ATP Content.

<sup>1</sup>Total of thirty-three substances: includes the 31 substances from the original validation study performed in one laboratory and the two interlaboratory validation studies (14 substances; two substances not among the 31 original substances assessed).

<sup>2</sup>K<sub>ow</sub> represents the estimated octanol-water partition coefficient (expressed on log scale) calculated by the Syracuse Research Corporation from the website: [http://www.syrres.com/esc/est\\_kowdemo.htm](http://www.syrres.com/esc/est_kowdemo.htm).

<sup>3</sup>Peptide reactivity based on Cys (1:10) and Lys (1:50) data as reported in Gerberick et al. (2007).

<sup>4</sup>Chemical classifications based on the Medical Subject Headings classification for chemicals and drugs, as developed by the National Library of Medicine: <http://www.nlm.nih.gov/mesh/meshhome.html>.

<sup>a</sup>Tested among the 31 substances used to assess the performance of the LLNA: DA (Daicel Chemical Industries, Ltd. 2007) and in the first interlaboratory validation study on LLNA: DA (Ikarashi et al. 2007).

<sup>b</sup>Tested among the 31 substances used to assess the performance of the LLNA: DA (Daicel Chemical Industries, Ltd. 2007) and in the second interlaboratory validation study on LLNA: DA (Kanazawa et al. 2007).

<sup>c</sup>Not tested among the 31 chemicals used to assess the performance of the LLNA: DA (Daicel Chemical Industries, Ltd. 2007) but in the first interlaboratory validation study on LLNA: DA (Ikarashi et al. 2007).