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**Appendix B**

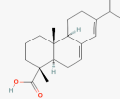


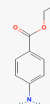



**Physico-Chemical Properties and Chemical Classes of Substances Tested in the  
LLNA: DA**

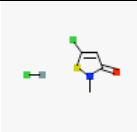
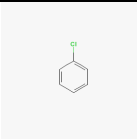
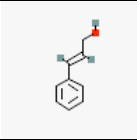
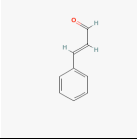
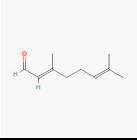

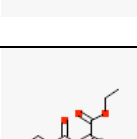
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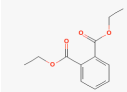
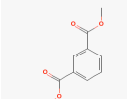
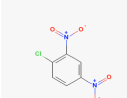
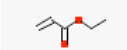
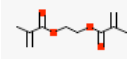
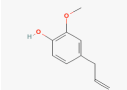
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
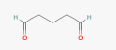

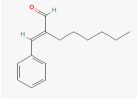
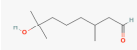
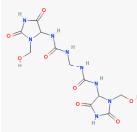
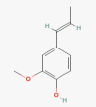
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





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

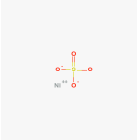
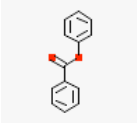
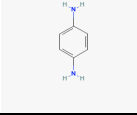
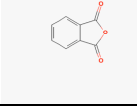

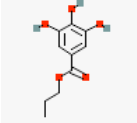
Substance Name <sup>1</sup>	Synonyms	CASRN	Mol. Weight (g/mol)	K <sub>ow</sub> <sup>2</sup>	Peptide Reactivity <sup>3</sup>	Physical Form	Chemical Class <sup>4</sup>	Structure
Abietic acid <sup>a, c</sup>	Sylvic acid	514-10-3	302.46	6.46	NA	Solid	Hydrocarbons, Cyclic; Polycyclic Compounds	
3-Aminophenol <sup>c</sup>	m-Aminophenol	591-27-5	109.13	0.24	Minimal	Solid	Amines; Phenols	
Benzalkonium chloride <sup>a</sup>	Alkylbenzyltrimethylammonium chloride; Germitol; Zephiral	8001-54-5	170.66	NA	NA	Solid/Liquid	Amines; Onium Compounds	
Benzocaine <sup>a</sup>	Ethyl 4-aminobenzoate	94-09-7	165.19	1.80	NA	Solid	Carboxylic Acids	
Benzoquinone <sup>b</sup>	p-Quinone 1,4-benzoquinone Cyclohexadienedione	106-51-4	108.10	1.17	High	Solid	Quinones	
1-Bromobutane <sup>a</sup>	Butyl bromide	109-65-9	137.02	2.65	Low	Liquid	Hydrocarbons, Halogenated	
Butyl glycidyl ether <sup>b</sup>	n- Butyl glycidyl ether	2426-08-6	130.19	1.42	NA	Liquid	Ethers	

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
5-Chloro-2-methyl-4-isothiazolin-3-one <sup>b</sup>	Chloromethylisothiazolinone CMI	26172-55-4	132.30	0.92	High	Liquid	Sulfur Compounds Heterocyclic Compounds	
Chlorobenzene <sup>a</sup>	Phenyl chloride	108-90-7	112.56	2.64	Minimal	Liquid	Hydrocarbons, Cyclic; Hydrocarbons, Halogenated	
Cinnamic alcohol <sup>b</sup>	3-Phenyl-2-propen-1-ol Cinnamyl alcohol	104-54-1	134.18	2.29	NA	Solid	Alcohols	
Cinnamic aldehyde <sup>a</sup>	Cinnamaldehyde	104-55-2	132.16	1.82	High	Liquid	Aldehydes	
Citral <sup>a</sup>	2,6-Octadienal, 3,7-dimethyl-	5392-40-5	152.24	3.45	High	Liquid	Hydrocarbons, Other	
Cobalt chloride <sup>a, c, d</sup>	Cobaltous chloride	7646-79-9	129.84	0.85	NA	Solid	Inorganic Chemical, Elements; Inorganic Chemical, Metals	
Diethyl maleate <sup>b</sup>	Ethyl maleate	141-05-9	172.18	0.89	High	Liquid	Carboxylic Acids	

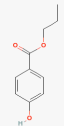



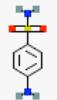
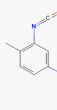
Substance Name <sup>1</sup>	Synonyms	CASRN	Mol. Weight (g/mol)	K <sub>ow</sub> <sup>2</sup>	Peptide Reactivity <sup>3</sup>	Physical Form	Chemical Class <sup>4</sup>	Structure
Diethyl phthalate <sup>a</sup>	Ethyl phthalate	84-66-2	222.24	2.65	Minimal	Liquid	Carboxylic Acids	
Dimethyl isophthalate <sup>b,c</sup>	1,3-Benzenedicarboxylic acid, dimethyl ester	1459-93-4	194.19	1.66	NA	Solid	Carboxylic Acids	
2,4-Dinitrochlorobenzene <sup>a,c</sup>	Dinitrochlorobenzene; DNCB	97-00-7	202.55	2.27	High	Solid	Hydrocarbons, Cyclic; Hydrocarbons, Halogenated; Nitro Compounds	
Ethyl acrylate <sup>b</sup>	2-Propenoic acid, ethyl ester	140-88-5	100.10	NA	High	Liquid	Carboxylic Acids	
Ethylene glycol dimethacrylate <sup>b</sup>	EGDMA	97-90-5	198.22	1.38	High	Liquid	Carboxylic Acids	
Eugenol <sup>a</sup>	2-Methoxy-4-(2-propenyl)phenol; Allylguaiacol	97-53-0	164.20	2.73	NA	Liquid	Carboxylic Acids	

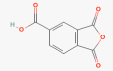
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Formaldehyde <sup>a, c</sup>	Formalin	50-00-0	30.03	0.35	Moderate	Liquid	Aldehydes	
Glutaraldehyde <sup>a, c</sup>	Glutaral; Pentanedial	111-30-8	100.12	-0.18	High	Liquid	Aldehydes	
Hexane <sup>a</sup>	Hexyl hydride; n-Hexane	110-54-3	86.18	3.29	Minimal	Liquid	Hydrocarbons, Acyclic	
Hexyl cinnamic aldehyde <sup>a, c, d</sup>	alpha-Hexylcinnamaldehyde; HCA	101-86-0	216.32	4.82	Minimal	Liquid	Aldehydes	
Hydroxycitronellal <sup>a</sup>	Citronellal hydrate	107-75-5	172.26	2.11	Low	Liquid	Hydrocarbons, Other	
Imidazolidinyl urea <sup>a</sup>	Germall 115; Imidurea	39236-46-9	388.30	-8.28	Moderate	Solid	Urea	
Isoeugenol <sup>a, c</sup>	2-Methoxy-4-propenylphenol; 4-Propenylguaiacol	97-54-1	164.20	2.65	NA	Liquid	Carboxylic Acids	

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, c</sup>	Isopropyl alcohol, 2-Propanol	67-63-0	60.10	0.28	Minimal	Liquid	Alcohols	
Lactic acid <sup>a, d</sup>	2-Hydroxypropanoic acid	50-21-5	90.08	-0.65	Minimal	Solid	Carboxylic Acids	
2-Mercaptobenzothiazole <sup>a</sup>	Captax	149-30-4	167.26	2.86	High	Solid	Heterocyclic Compounds	
Methyl methacrylate <sup>b</sup>	MMA	80-62-6	100.12	NA	NA	Liquid	Carboxylic Acids	
Methyl salicylate <sup>a, c</sup>	Oil of wintergreen; Methyl 2-hydroxybenzoate	119-36-8	152.15	2.60	Minimal	Liquid	Carboxylic Acids; Phenols	
Nickel (II) chloride <sup>b</sup>	Nickel chloride	7718-54-9	129.60	NA	NA	Solid	Inorganic Chemical, Elements; Inorganic Chemical, Metals	

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
Nickel (II) sulfate hexahydrate <sup>a, c, d</sup>	Nickel sulfate hexahydrate	10101-97-0	154.76	NA	NA	Solid	Inorganic Chemical, Elements; Inorganic Chemical, Metals	
Phenyl benzoate <sup>b</sup>	Diphenylcarboxylate	93-99-2	198.22	2.89	NA	Solid	Carboxylic Acids	
p-Phenylenediamine <sup>a</sup>	4-Phenylenediamine	106-50-3	108.14	-0.39	NA	Solid	Amines	
Phthalic anhydride <sup>a</sup>	1,2-Benzenedicarboxylic anhydride; 1,3-Dioxophthalan	85-44-9	148.12	2.07	Moderate	Solid	Anhydrides; Carboxylic Acids	
Potassium dichromate <sup>a,d</sup>	PDC; Dipotassium bichromate	7778-50-9	294.18	-3.59	NA	Solid	Inorganic Chemical, Chromium Compounds; Inorganic Chemical, Potassium Compounds	
Propyl gallate <sup>b</sup>	Benzoic acid, 3,4,5-trihydroxy-, propyl ester; Gallic acid, propyl ester;	121-79-9	212.20	NA	High	Solid	Carboxylic Acids	



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
	Propyl 3,4,5-trihydroxybenzoate							
Propylparaben <sup>a</sup>	4-Hydroxybenzoic acid, propyl ester; Propyl p-hydroxybenzoate	94-13-3	180.20	2.98	Minimal	Solid	Carboxylic Acids; Phenols	
Resorcinol <sup>a</sup>	1,3-Dihydroxybenzene	108-46-3	110.11	1.03	Minimal	Solid	Phenols	
Salicylic acid <sup>b</sup>	2-Hydroxybenzoic acid	69-72-7	138.12	1.03	NA	Solid	Phenols; Carboxylic Acids	
Sodium lauryl sulfate <sup>a</sup>	Sodium dodecyl sulfate, SLS, SDS, Irium	151-21-3	288.38	1.69	NA	Solid	Alcohols; Sulfur Compounds; Lipids	
Sulfanilamide <sup>b</sup>	4-Aminobenzene-sulfonamide, p-Anilinesulfonamide, p-Sulfamidoaniline	63-74-1	172.21	0.40	Minimal	Solid	Hydrocarbons, Cyclic; Sulfur Compounds	
Toluene 2,4-diisocyanate <sup>a</sup>	2,4-TDI	584-54-9	174.16	3.74	NA	Liquid	Hydrocarbons, Cyclic; Isocyanates	

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
Trimellitic anhydride <sup>a</sup>	4-Carboxyphthalic anhydride	552-30-7	192.13	1.95	Low	Solid	Anhydride; Carboxylic Acids	

31 Abbreviations: CASRN = Chemical Abstracts Service Registry Number; K<sub>ow</sub> = octanol-water partition coefficient; Mol. = molecular; LLNA: DA = murine local  
 32 lymph node assay modified by Daicel Chemical Industries, Ltd. based on ATP content; NA = not available.

33 <sup>1</sup>Total of 46 substances: intralaboratory validation study tested 45 substances (Idehara et al. 2008; Idehara unpublished data) and the two-phased interlaboratory  
 34 validation study tested 13 of the 45 substances from the intralaboratory validation study and one substance not previously evaluated.

35 <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:  
 36 [http://www.syrres.com/esc/est\\_kowdemo.htm](http://www.syrres.com/esc/est_kowdemo.htm).

37 <sup>3</sup>Peptide reactivity based on Cys (1:10) and Lys (1:50) data as reported in Gerberick et al. 2004 and/or Gerberick et al. 2007.

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

40 <sup>a</sup>Substance tested in intralaboratory validation study (Idehara et al. 2008).

41 <sup>b</sup>Substance tested in intralaboratory validation study (Idehara unpublished data).

42 <sup>c</sup>Substance tested in phase one of two-phased interlaboratory validation study (Omori et al. 2008).

43 <sup>d</sup>Substance tested in phase two of two-phased interlaboratory validation study (Omori et al. 2008).