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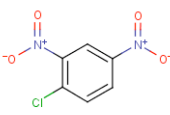
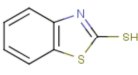

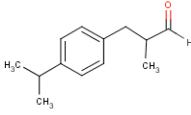
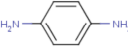
Appendix B

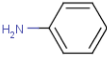
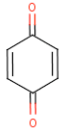
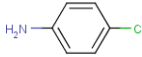
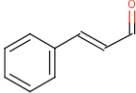
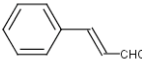
Physico-Chemical Properties of Substances Tested Using the LLNA: BrdU-ELISA

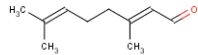
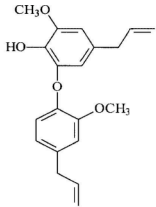
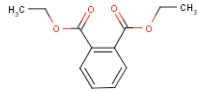
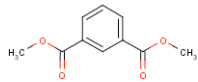
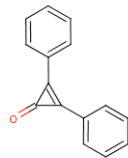
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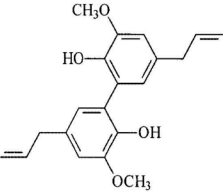
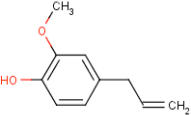


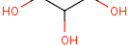
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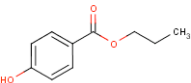
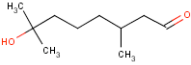
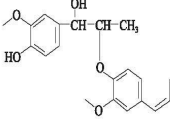
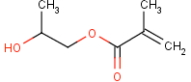
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30**Appendix B Physicochemical Characteristics of Substances Tested in the LLNA: BrdU-ELISA (Alphanumeric Order)**

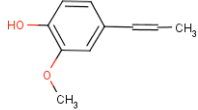

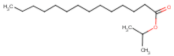
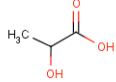
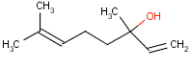
Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow ^{1,2}	Peptide Reactivity ³	Physical Form	Chemical Class ⁴	Structure
1-Chloro-2-dinitrobenzene	2,4-Dinitrochlorobenzene	97-00-7	202.55	-0.057	High	Solid	Hydrocarbon, halogenated; Nitro compounds; Hydrocarbons, cyclic	
2-Mercaptobenzothiazole	Captax	149-30-4	167.253	1.8	High	Solid	Heterocyclic compounds	
3-Aminophenol	m-Aminophenol; 3-Hydroxyaniline	591-27-5	109.126	1.17	NA	Solid	Amines; Phenols	
3-(4-Isopropylphenyl) isobutyraldehyde	Cyclamen aldehyde	103-95-7	190.28	3.28	Low	Liquid	Carboxylic acids	
1,4-Phenylenediamine	p-PDA; p-Phenylenediamine	106-50-3	108.141	1.17	NA	Solid	Amines	

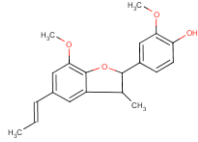
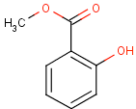
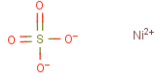
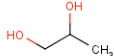
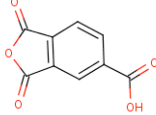
Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow ^{1,2}	Peptide Reactivity ³	Physical Form	Chemical Class ⁴	Structure
Aniline	Benzenamine	62-53-3	93.1265	1.56	NA	Liquid	Amines	
Benzoquinone	p-Quinone; 1,4-Cyclohexadienedione	106-51-4	108.095	1.17	High	Solid	Quinones	
4-Chloroaniline	4-Chlorobenzeneamine; Aniline, p-chloro-; Benzenamine, 4-chloro-	106-47-8	127.57	1.8	NA	Liquid	Amines	
<i>trans</i> -Cinnamaldehyde	3-Phenylpropenal	14371-10-9	132.6	1.82	NA	Liquid	Aldehydes	
Cinnamic aldehyde	Cinnamal; cinnamaldehyde; 3-phenyl-2-propenal	104-55-2	132.16	2.29	High	Liquid	Aldehydes	

Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow ^{1,2}	Peptide Reactivity ³	Physical Form	Chemical Class ⁴	Structure
Citral	3,7-Dimethyl-2,6-octadienal; Geranial-neral mixture	5392-40-5	152.233	2.54/ 3.45	NA	Liquid	Hydrocarbons, other	
4,5'-Diallyl-2'-hydroxy-2,3'-dimethoxyphenyl ether	DHEB	NA	326.39	NA	NA	NA	Carboxylic acids	
Diethyl phthalate	1,2-Benzenedicarboxylic acid, diethyl ester; Diethyl 1,2-benzenedicarboxylate	84-66-2	222.24	1.87	Minimal	Liquid	Carboxylic acids	
Dimethyl isophthalate	Dimethyl m-phthalate	1459-93-4	194.19	1.66	NA	Solid	Carboxylic acids	
Diphenylcyclopropenone	2,3-Diphenylcyclopropenone	886-38-4	206.24	3.25	High	Solid	Hydrocarbons, cyclic	

Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow ^{1,2}	Peptide Reactivity ³	Physical Form	Chemical Class ⁴	Structure
2,2'-Dihydroxyl-3,3'-dimethoxy-5,5'-diallyl-biphenyl	DHEA	NA	326.39	NA	NA	NA	Carboxylic acids	
Eugenol	2-Methoxy-4-(2-propenyl)phenol; 4-Allyl-2-methoxyphenol; 4-Allylguaiacol	97-53-0	164.201	2.15/ 2.73	NA	Liquid	Carboxylic acids	
Formaldehyde	Formalin	50-00-0	30.03	0.33	Moderate	Liquid	Aldehydes	
Glutaraldehyde	Glutaral	111-30-8	100.12	0.92	High	Liquid	Aldehydes	
Glycerol	Glycerin	56-81-5	92.09	0.05	Minimal	Liquid	Alcohols; Carbohydrates	

Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow ^{1,2}	Peptide Reactivity ³	Physical Form	Chemical Class ⁴	Structure
Hexane	Hexyl hydride; n-Hexane	110-54-3	86.1754	1.94	Minimal	Liquid	Hydrocarbons, acyclic	
Hexyl cinnamic aldehyde	HCA; alpha-Hexylcinnamaldehyde; 2-(Phenylmethylene)octanal	101-86-0	216.319	3.77/ 4.82	Minimal	Liquid	Aldehydes	
Hydroxycitronellal	7-Hydroxy-3,7-dimethyloctanol	107-75-5	172.26	2.15	Low	Liquid	Hydrocarbons, other	
4-[1-Hydroxy-2-(2-methoxy-4-propenylphenoxy)-propyl]-2-methoxy-phenol	□-O-4-Dilignol	NA	327.39	NA	NA	NA	Carboxylic acids	
2-Hydroxypropyl methacrylate	2-HPMA	923-26-2	144.168	1.03	Low	Solid	Carboxylic acids	

Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow ^{1,2}	Peptide Reactivity ³	Physical Form	Chemical Class ⁴	Structure
Isoeugenol	2-Methoxy-4-propenylphenol; 4-Propenylguaiacol	97-54-1	164.201	2.15	NA	Liquid	Carboxylic acids	
Isopropanol	Isopropyl alcohol, 2-Propanol	67-63-0	60.095	0.82	Minimal	Liquid	Alcohols	
Isopropyl myristate	1-Methylethyl tetradecanoate	110-27-0	270.46	3.88	Minimal	Liquid	Lipids	
Lactic acid	2-Hydroxypropanoic acid	50-21-5	90.08	0.05	Minimal	Liquid	Carboxylic acids	
Linalool	3,7-dimethylocta-,6-dien-3-ol	78-70-6	154.25	2.54	NA	Liquid	Hydrocarbons	

Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow ^{1,2}	Peptide Reactivity ³	Physical Form	Chemical Class ⁴	Structure
2-Methoxy-4-(7-methoxy-3-methyl-5-propenyl-2,3-dihydro-benzofuran-2yl)-phenol	Dehydrodiisoeugenol	2680-81-1	326.39	NA	NA	NA	Carboxylic acids	
Methyl salicylate	Oil of wintergreen; 2-Hydroxybenzoic acid methyl ester	119-36-8	152.15	1.28	Minimal	Liquid	Phenols; Carboxylic acids	
Nickel Sulfate	Nickelous sulfate	7786-81-4	154.76	NA	NA	Solid	Inorganic chemicals, metals; Inorganic chemicals, elements	
Propylene glycol	1,2-Dihydroxypropane; 1,2-Propanediol	57-55-6	76.0944	0.43	Minimal	Liquid	Alcohols	
Trimellitic anhydride	1,2,4-Benzenetricarboxylic acid, cyclic 1,2-anhydride (8CI); 1,3-Dihydro-1,3-dioxo-5-isobenzofuran-carboxylic acid; 5-Isobenzofuran-carboxylic acid; 1,3-dihydro-1,3-dioxo-Benzene-1,2,4-tricarboxylic acid 1,2-anhydride	552-30-7	192.13	1.95	Low	Solid	Anhydrides, Carboxylic acids	

31 Abbreviations: CASRN=Chemical Abstracts Registry Number; g/mol=grams per mole; NA = Not available.
32 ¹Physicochemical properties were obtained from PubChem (<http://pubchem.ncbi.nlm.nih.gov/>), ChemID (<http://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp>), or the Sigma Chemical
33 Catalog.
34 ²K_{ow} represents the octanol-water partition coefficient (expressed on log scale). When two numbers are shown, the first number is the value calculated by the method of Moriguchi et al.
35 (1994 Chem Pharm Bull. 42:976-978) and provided in Gerberick et al. (2005 Dermatitis. 16:157-202). The second number was calculated by the method of Meylan and Howard (1995
36 J Pharm Science. 84:83-92) and obtained from the website: http://www.syrres.com/esc/est_kowdemo.htm.
37 ³Peptide reactivity data obtained from: Gerberick et al. 2007.
38 ⁴Chemical classifications based on the Medical Subject Headings classification for chemicals and drugs developed by the National Library of Medicine found at
39 <http://www.nlm.nih.gov/mesh/meshhome.html>.
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