APPENDIX C

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

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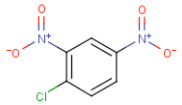
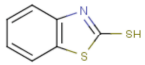
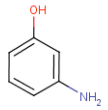
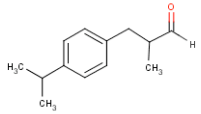
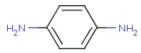
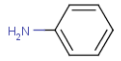
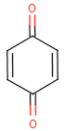
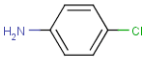
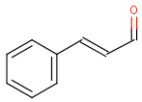
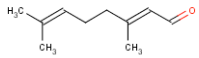
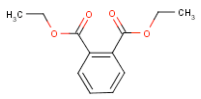
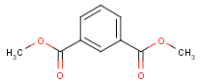
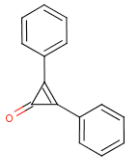
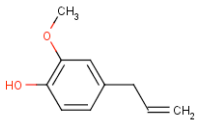
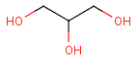
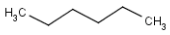
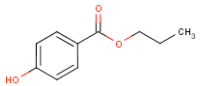
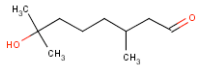
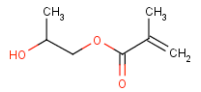
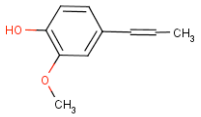
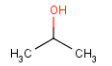
Appendix C Physicochemical Characteristics of Substances Tested in the LLNA: BrdU-ELISA (Alphanumeric Order)

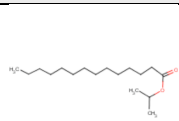
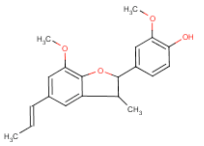
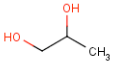
Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow[1,2]	Peptide Reactivity[3]	Physical Form	Chemical Class[4]	Structure
1-Chloro-2-dinitrobenzene	Dinitrochlorobenzene	97-00-7	202.55	-0.057	High	Solid	Hydrocarbon, Halogenated; Nitro Compounds; Hydrocarbons, Cyclic	
2-Mercaptobenzothiazole	Captax	149-30-4	167.253	1.8	High	Solid	Heterocyclic Compounds	
3-Aminophenol	m-Aminophenol; 3-Hydroxyaniline	591-27-5	109.126	1.17		Solid	Amines; Phenols	
3-(4-Isopropylphenyl) isobutyraldehyde	Cyclamen aldehyde	103-95-7	190.28	NA	Low	Liquid	Carboxylic acids	
4-Phenylenediamine	p-PDA, p-Phenylenediamine	106-50-3	108.141	1.17		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		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		Liquid	Amines	
trans-Cinnamaldehyde	3-Phenylpropenal	14371-10-9	132.6	1.82		Liquid	Aldehydes	
Citral	3,7-Dimethyl-2,6-octadienal; Geranial-Neral mixture	5392-40-5	152.233	2.54/ 3.45		Liquid	Hydrocarbons, Other	

Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow[1,2]	Peptide Reactivity[3]	Physical Form	Chemical Class[4]	Structure
4,5'-Diallyl-2'-hydroxy-2,3'-dimethoxyphenyl ether	DHEB	NA	NA	NA		NA	NA	NA
Diethylpthalate	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		Solid	Carboxylic Acids	
Diphenylcyclopropenone	2,3-Diphenylcyclo-propenone	886-38-4	206.24	3.25	High	Solid	Hydrocarbons, Cyclic	
2,2'-Dihydroxyl-3,3'-dimethoxy-5,5'-diallyl-biphenyl	DHEA	NA	NA	NA		NA	NA	NA

Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow[1,2]	Peptide Reactivity[3]	Physical Form	Chemical Class[4]	Structure
Eugenol	2-Methoxy-4-(2-propenyl)phenol; 4-Allyl-2-methoxyphenol; 4-Allylguaiacol	97-53-0	164.201	2.15/ 2.73		Liquid	Carboxylic Acids	
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	
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	

Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow[1,2]	Peptide Reactivity[3]	Physical Form	Chemical Class[4]	Structure
Hydroxycitronellal	7-Hydroxy-3,7-dimethyloctanol	107-75-5	172.26	2.15	Low	Liquid	Hydrocarbons, Other	
4-[1-Hydroxy-2-(2-methoxy-4-propenyl-phenyoxy)-propyl]-2-methoxy-phenol	□-O-4-Dilignol	NA	327.39	NA		NA	NA	NA
2-Hydroxypropyl methacrylate	2-HPMA	923-26-2	144.168	1.03	Low	Solid	Carboxylic Acids	
Isoeugenol	2-Methoxy-4-propenylphenol; 4-Propenylguaiacol	97-54-1	164.201	2.15		Liquid	Carboxylic Acids	
Isopropanol	Isopropyl alcohol, 2-Propanol	67-63-0	60.095	0.82	Minimal	Liquid	Alcohols	

Chemical Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log Kow[1,2]	Peptide Reactivity[3]	Physical Form	Chemical Class[4]	Structure
Isopropyl myristate	1-Methylethyl tetradecanoate	110-27-0	270.46	3.88	Minimal	Liquid	Lipids	
2-Methoxy-4-(7-methoxy-3-methyl-5-propenyl-2,3-dihydro-benzofuran-2yl)-phenol	Dehydrodiisoeugenol	2680-81-1	326.39	NA		NA	NA	
Propylene glycol	1,2-Dihydroxypropane; 1,2-Propanediol	57-55-6	76.0944	0.43	Minimal	Liquid	Alcohols	

Abbreviations: CASRN=Chemical Abstracts Registry Number; g/mol=grams per mole; NA = Not available.
[1]Physicochemical 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 Catalog.
[2]K_{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. (1994 Chem Pharm Bull. 42:976-978) and provided in Gerberick et al. (2005 Dermatitis. 16:157-2002). The second number was calculated by the method of Meylan and Howard (1995 J Pharm Science. 84:83-92) and obtained from the website: http://www.syrres.com/esc/est_kowdemo.htm.
[3]Peptide reactivity data obtained from: Gerberick et al. 2007
[4]Chemical classifications based on the Medical Subject Headings classification for chemicals and drugs developed by the National Library of Medicine found at http://www.nlm.nih.gov/mesh/meshhome.html.