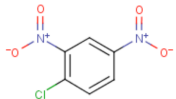
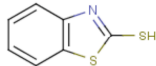
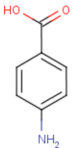
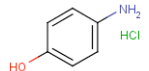

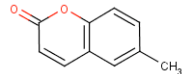
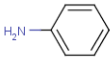
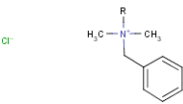
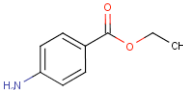
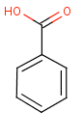


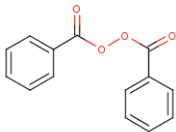

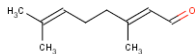
APPENDIX B

Physico-Chemical Properties Substances Tested Using the LLNA: BrdU-FC and the eLLNA: BrdU-FC Protocol

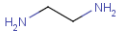
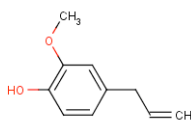
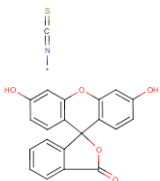

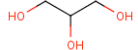
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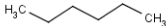
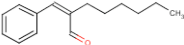
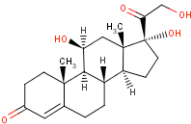
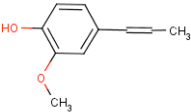

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Kow ¹	Peptide Reactivity ²	Physical Form	Chemical Class ³	Structure
2, 4-Dinitrochlorobenzene	Dinitrochlorobenzene; DNCB	97-00-7	203	2.27	High	Solid	Hydrocarbon, Halogenated; Nitro Compounds; Hydrocarbons, Cyclic	
2-Mercaptobenzothiazole	Captax	149-30-4	167	2.86	High	Solid	Heterocyclic compounds	
4-Aminobenzoic acid	PABA	150-13-0	137	0.83	NA	Solid	Carboxylic Acids	
4-Aminophenol HCl	4-Hydroxyanilinium chloride	51-78-5	145	NA	NA	Solid	Amines; Phenols	
4-Phenylenediamine	p-Phenylenediamine	106-50-3	108	-0.39	NA	Solid	Amines	

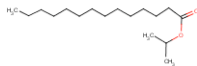
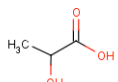
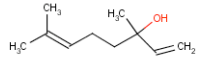


Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Kow ¹	Peptide Reactivity ²	Physical Form	Chemical Class ³	Structure
6-Methylcoumarin	6-MC	92-48-8	160	2.15	Minimal	Solid	Heterocyclic Compounds	
Aniline	Benzenamine	62-53-3	93.1	1.56	NA	Liquid	Amines	
Benzalkonium chloride	Alkylbenzyltrimethyl ammonium chloride; Germitol; Zephiral	8001-54-5	171	NA	NA	Solid/Liquid	Onium Compounds	
Benzocaine	Ethyl 4-aminobenzoate	94-09-7	165	1.8	NA	Solid	Carboxylic Acids	
Benzoic acid	Benzenecarboxylic acid Benzeneformic acid Benzenemethanoic acid Benzoate	65-85-0	212	1.87	NA	Solid	Carboxylic Acids	

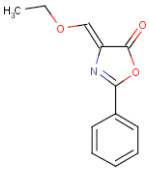
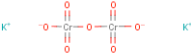
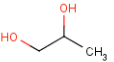
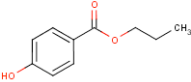

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Kow ¹	Peptide Reactivity ²	Physical Form	Chemical Class ³	Structure
Benzoyl peroxide	Dibenzoyl peroxide	94-36-0	242	3.46	High	Solid	Carboxylic acids	
Chlorobenzene	Phenyl chloride	108-90-7	113	2.64	Minimal	Liquid	Hydrocarbons, Cyclic; Hydrocarbons, Halogenated	
Chlorpromazine + UVR	NA	NA	NA	NA	NA	NA	Sulfur Compounds; Heterocyclic Compounds	NA
Citral	2,6-Octadienal, 3,7-dimethyl-	5392-40-5	152	3.45	NA	Liquid	Hydrocarbons, Other	
Cobalt chloride	Cobaltous chloride	7646-79-9	130	0.85	NA	Solid	Inorganic chemicals, Metals; Elements	$[Cr]_2^*$ $[Co^{2+}]$

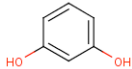
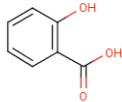
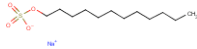
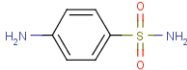
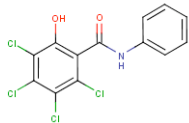
Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Kow ¹	Peptide Reactivity ²	Physical Form	Chemical Class ³	Structure
Copper chloride	NA	1344-67-8	99.0	NA	NA	Solid	Inorganic chemicals, Elements	
Croton oil	Croton resin	8001-28-3	NA	NA	NA	Liquid	Lipids	NA
Diethylenetriamine	1,2-Ethanediamine, N-(2-aminoethyl)-	111-40-0	103	0.29	NA	Liquid	Amines	
Diphenylcyclopropenone	2,3-Diphenylcyclopropenone	886-38-4	206	3.25	High	Solid	Hydrocarbons, Cyclic	
Ethylene glycol dimethacrylate	EGDMA	97-90-5	198	1.38	High	Liquid	Carboxylic Acids	

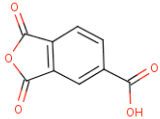

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Kow ¹	Peptide Reactivity ²	Physical Form	Chemical Class ³	Structure
Ethylenediamine	1,2-Diaminoethane	107-15-3	60.1	-2.04		Liquid	Amines	
Eugenol	2-Methoxy-4-(2-propenyl)phenol; Allylguaiacol	97-53-0	164	2.73		Liquid	Carboxylic Acids	
Fluorescein isothiocyanate	FITC	27072-45-3	389	3.32	High	Solid	Polycyclic Compounds; Isocyanates; Sulfur Compounds	
Formaldehyde	Formalin	50-00-0	30.0	0.35	Moderate	Liquid	Aldehydes	
Glycerol	Glycerin	56-81-5	92.1	0.05	Minimal	Liquid	Alcohols; Carbohydrates	

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Kow ¹	Peptide Reactivity ²	Physical Form	Chemical Class ³	Structure
Hexane	Hexyl hydride; n-Hexane	110-54-3	86.2	3.29	Minimal	Liquid	Hydrocarbons, Acyclic	
Hexyl cinnamic aldehyde	alpha-Hexylcinnamaldehyde; HCA	101-86-0	216	4.82	Minimal	Liquid	Aldehydes	
Hydrocortisone	11-beta-Hydrocortisone	50-23-7	362	1.16		Solid	Polycyclic Compounds	
Isoeugenol	2-Methoxy-4-propenylphenol; 4-Propenylguaiacol	97-54-1	164	2.65		Liquid	Carboxylic acids	
Isopropanol	Isopropyl alcohol, 2-Propanol	67-63-0	60.1	0.28	Minimal	Liquid	Alcohols	

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Kow ¹	Peptide Reactivity ²	Physical Form	Chemical Class ³	Structure
Isopropyl myristate	1-Methylethyl tetradecanoat	110-27-0	270	3.88	Minimal	Liquid	Lipids	
Lactic acid	2-Hydroxypropanoic acid	50-21-5	90.1	-0.65	Minimal	Solid	Carboxylic Acids	
Linalool	3,7-dimethylocta-,6-dien-3-ol	78-70-6	154	2.97		Liquid	Hydrocarbons	
Methyl salicylate	Oil of wintergreen; Methyl 2-hydroxybenzoate	119-36-8	152	2.6	Minimal	Liquid	Phenols; Carboxylic Acids	
Nickel chloride	Nickel dichloride	7718-54-9	129	NA		Solid	Inorganic chemicals, Elements	

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Kow ¹	Peptide Reactivity ²	Physical Form	Chemical Class ³	Structure
Oxazalone	4-Ethoxymethylene-2-phenyloxazol-5-one	15646-46-5	217	1.87	High	Solid	Heterocyclic Compounds	
Potassium dichromate	PDC; Dipotassium bichromate	7778-50-9	294	-3.59		Solid	Inorganic Chemical, Chromium Compounds; Potassium Compounds	
Propylene glycol	1,2-Dihydroxypropane; 1,2-Propanediol	57-55-6	76.1	0.43	Minimal	Liquid	Alcohols	
Propylparaben	4-Hydroxybenzoic acid, propyl ester; Propyl p-hydroxybenzoate	94-13-3	180	2.98	Minimal	Solid	Phenols; Carboxylic Acids	
Pyridine	Azabenzene	110-86-1	79.1	1.31	NA	Liquid	Heterocyclic Compounds	

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Kow ¹	Peptide Reactivity ²	Physical Form	Chemical Class ³	Structure
Resorcinol	1,3-Dihydroxybenzene	108-46-3	110	1.03	Minimal	Solid	Phenols	
Salicylic acid	2-Hydroxybenzoic acid	69-72-7	138	1.03	NA	Solid	Phenols; Carboxylic Acids	
Sodium lauryl sulfate	Sodium dodecyl sulfate, SLS, SDS, Irium	151-21-3	288	1.69	NA	Solid	Alcohols; Sulfur Compounds; Lipids	
Sulfanilimide	4-Aminobenzenesulfonamide; p-Anilinesulfonamide; p-Sulfamidoaniline	63-74-1	172	0.4	Minimal	Solid	Amides; Sulfur Compounds; Amines	
Tetrachlorosalicylanilide	NA	7426-07-5	351	NA	Moderate	Solid	Amides; Amines	

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Kow ¹	Peptide Reactivity ²	Physical Form	Chemical Class ³	Structure
Trimellitic anhydride	4-Carboxyphthalic anhydride	552-30-7	192	1.95	Low	Solid	Anhydrides; Carboxylic Acids	
Tween 80	Polyethylene glycol sorbitan monooleate Polyoxyethylene sorbitan monooleate Polysorbate 80	9005-65-6	1310	NA	NA	Liquid	Alcohols	NA
Xylene	Dimethylbenzene	1330-20-7	107	3.16	NA	Liquid	Hydrocarbons, Cyclic	

Abbreviations: CASRN = Chemical Abstract Services Registry Number; g/mol = grams per mole; Mol. = Molecular; NA = Not available.

¹Kow 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.

²Peptide reactivity data obtained from: Gerberick et al. 2007. Quantification of chemical peptide reactivity for screening contact allergens: A classification tree model approach. Toxicol Sci 97:417-427.

³Chemical 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>.