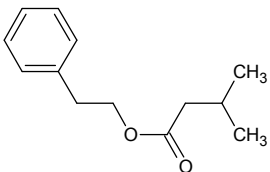
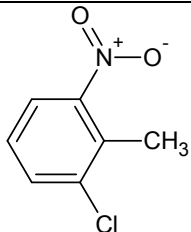
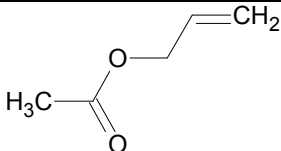
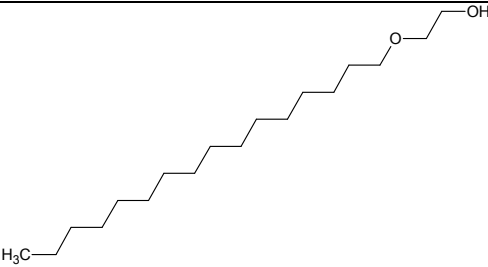
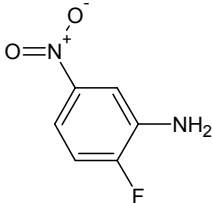
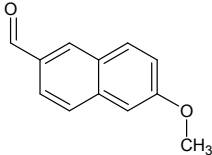
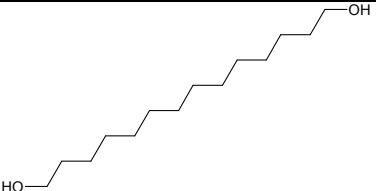
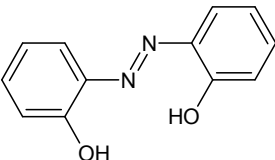
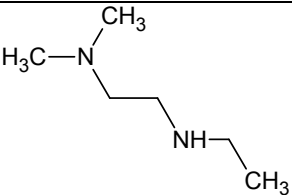
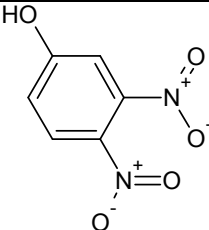
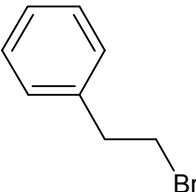
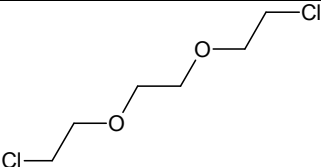
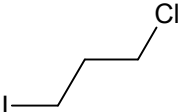


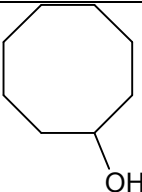
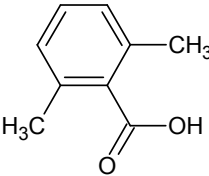
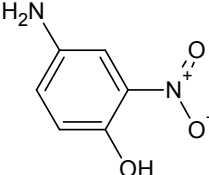
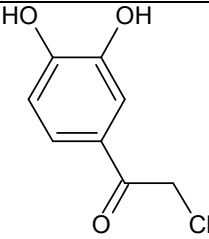
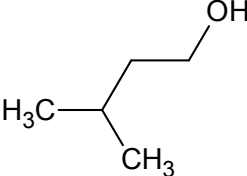
Supporting Information

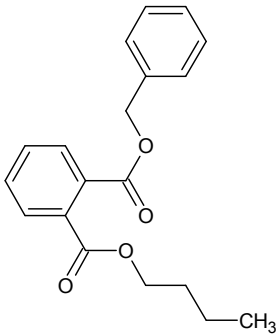
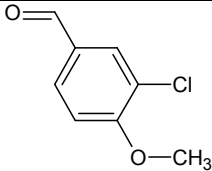
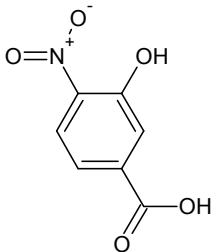
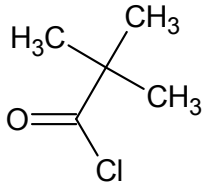
Table of the validation dataset of 40 chemicals tested in the LLNA

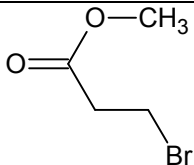
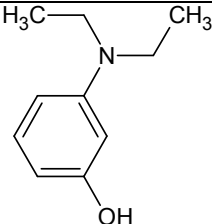
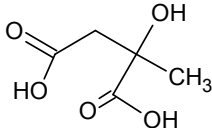
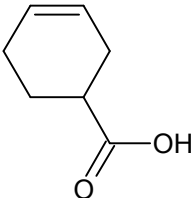
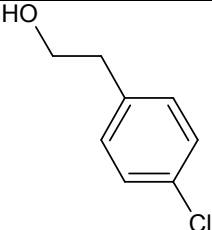
NAME	CASRN	STRUCTURE	EC3%	Sensitization Potency Classification	LLNA Outcome	TIMES-SS Outcome
butanoic acid, 3-methyl-, 2-phenylethyl ester (2-phenylethyl 3-methylbutanoate)	140-26-1		39.5	Weak sensitizer	Pos	Neg
2-chloro-6-nitrotoluene	83-42-1		NC	Non-sensitizer	Neg	Neg
allyl acetate	591-87-7		NC	Non-sensitizer	Neg	Pos

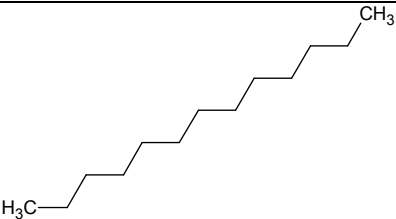
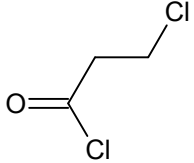
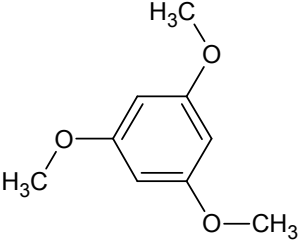
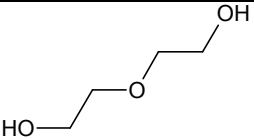
2-(hexadecyloxy)ethanol	2136-71-2		8.8	Moderate sensitizer	Pos	Neg
2-fluoro-5-nitroaniline	69-36-8		NC	Non-sensitizer	Neg	Pos
6-methoxynaphthalene-2-carbaldehyde	3453-33-6		NC	Non-sensitizer	Neg	Neg
tetradecane-1,14-diol	19812-64-7		NC	Non-sensitizer	Neg	Neg
2,2'-azobis-phenol	2050-14-8		27.9	Weak sensitizer	Pos	Pos

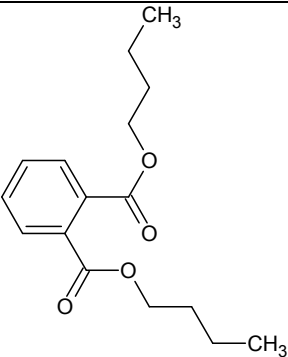
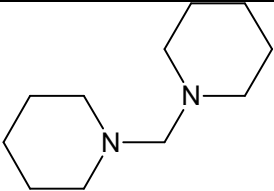
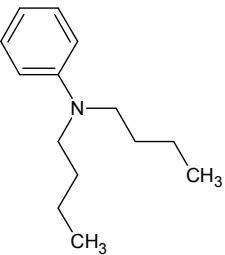
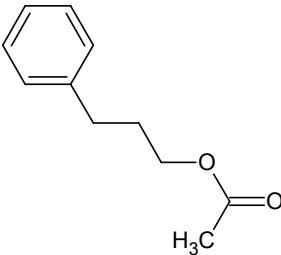
2-ethylaminoethyl dimethylamine	123-83-1		11.3	Weak sensitizer	Pos	Pos
3,4-dinitrophenol	577-71-9		NC	Moderate sensitizer	Pos	Neg
2-bromoethyl benzene	103-63-9		6.2	Moderate sensitizer	Pos	Neg
1,2-bis(2-chloroethoxy)-ethane	112-26-5		NC	Non-sensitizer	Neg	Pos
1-chloro-3-iodopropane	6940-76-7		NC	Non-sensitizer	Neg	Neg

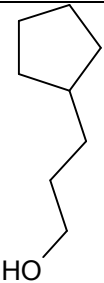
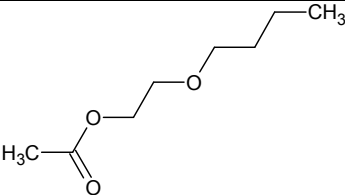
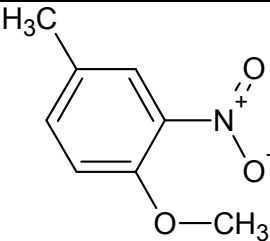
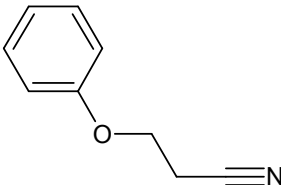
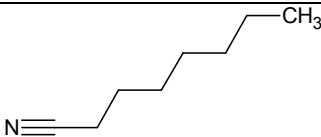
cyclooctanol	696-71-9		NC	Non-sensitizer	Neg	Neg
2,6-dimethylbenzoic acid	632-46-2		NC	Non-sensitizer	Neg	Neg
4-amino-2-nitrophenol	119-34-6		NC	Strong sensitizer	Pos	Pos
2-chloro-3',4'-dihydroxyacetophenone	99-40-1		NC	Strong extreme	Pos	Pos
3-methyl-1-butanol	123-51-3		NC	Non-sensitizer	Neg	Neg

butylbenzylphthalate	85-68-7		NC	Non-sensitizer	Neg	Neg
3-chloro-p-anisaldehyde	4903-09-7		NC	Non-sensitizer	Neg	Neg
3-hydroxy-4-nitrobenzoic acid	619-14-7		NC	Non-sensitizer	Neg	Neg
2,2-dimethyl propanoyl chloride	3282-30-2		NC	Moderate sensitizer	Pos	Pos

propanoic acid, 3-bromo-, methyl ester (methyl 3-bromopropanoate)	3395-91-3		NC	Non-sensitizer	Neg	Neg
3-(diethylamino)-phenol	91-68-9		NC	Moderate sensitizer	Pos	Pos
(s)-2-hydroxy-2-methylsuccinic acid	6236-09-5		NC	Non-sensitizer	Neg	Neg
cyclohex-3-ene-1-carboxylic acid	4771-80-6		9.3	Moderate sensitizer	Pos	Pos
p-chlorophenethylic alcohol	1875-88-3		31.3	Weak sensitizer	Pos	Neg

tridecane	629-50-5		48.4	Weak sensitizer	Pos	Neg
3-chloropropionyl chloride	625-36-5		NC	Strong extreme	Pos	Pos
1,3,5-trimethoxy-benzene	621-23-8		NC	Non-sensitizer	Neg	Neg
2,2'-oxybisethanol	111-46-6		NC	Non-sensitizer	Neg	Neg

1,2-benzenedicarboxylic acid, dibutyl ester (dibutyl phthalate)	84-74-2		NC	Non-sensitizer	Neg	Neg
dipiperidinomethane	880-09-1		NC	Strong sensitizer	Pos	Pos
N,N-dibutylaniline	613-29-6		19. 6	Weak sensitizer	Pos	Neg
3-phenylpropyl acetate	122-72-5		NC	Non-sensitizer	Neg	Neg

cyclopentanepropanol (3-cyclopentylpropan-1-ol)	767-05-5		NC	Non-sensitizer	Neg	Neg
ethanol, 2-butoxy-, acetate (2-butoxyethyl acetate)	112-07-2		NC	Non-sensitizer	Neg	Neg
1-methoxy-4-methyl-2-nitro-benzene	119-10-8		NC	Non-sensitizer	Neg	Neg
3-phenoxypropionitrile	3055-86-5		NC	Non-sensitizer	Neg	Neg
octanenitrile	124-12-9		NC	Non-sensitizer	Neg	Neg

