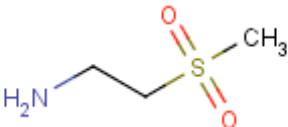
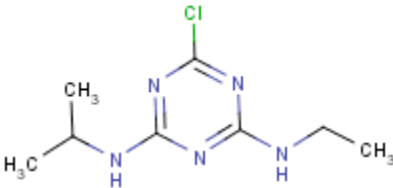

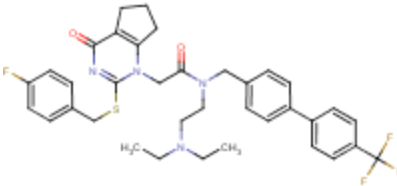



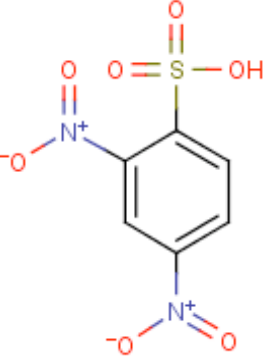
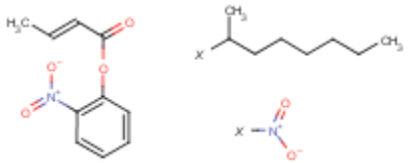
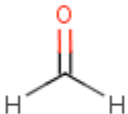
APPENDIX D1


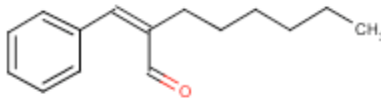
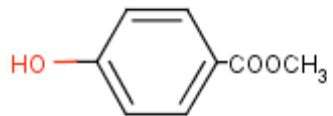
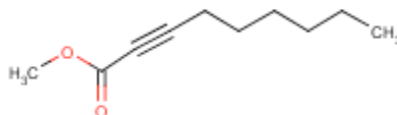
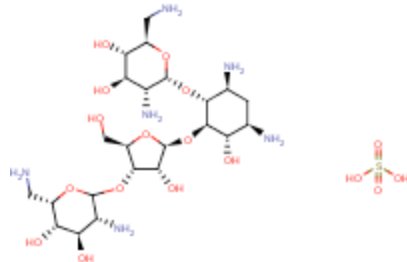
Physico-Chemical Properties and Chemical Classes of Substances Tested in Aqueous Solutions Analyzed in the Applicability Domain of the LLNA

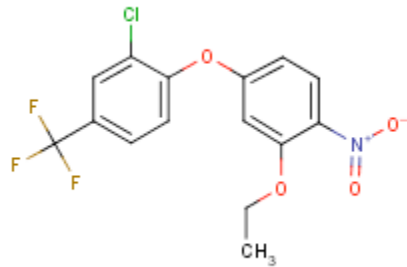
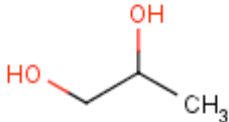
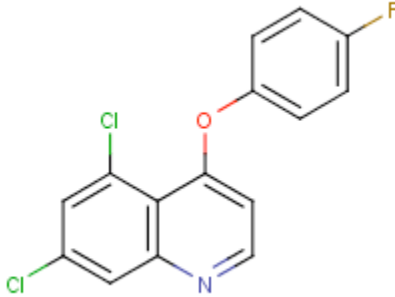
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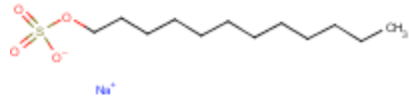
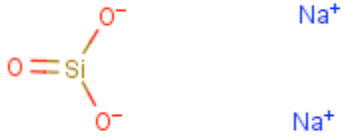
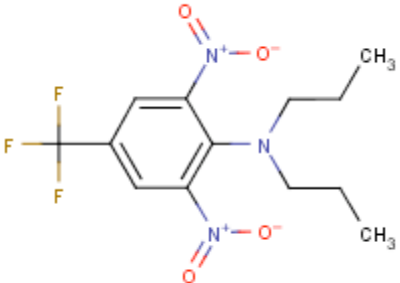
Physico-Chemical Properties – Substances Tested in Aqueous Solutions (Sorted Alphabetically)

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow ¹	Physical Form	Chemical Class ²	Structure ³
2-Aminoethyl methylsulfone	NA	49773-20-8	123.18	NA	Solid	Sulfur Compounds	
Atrazine SC	Atrazine; 1-Chloro-3-ethylamino-5-isopropylamino-2,4,6-triazine	1912-24-9	215.69	2.82	Solid	Heterocyclic Compounds	
1-Butanol	n-Butanol	71-36-3	74.12	0.84	Liquid	Alcohols; Lipids	
n-[2-(diethylamino)ethyl]-2-[[[4-(4-fluorophenyl)methyl]thio]-4,5,6,7-tetrahydro-4-oxo-n-[[4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl]methyl]-1h-cyclopentapyrimidine-1-acetamide	Darapladib	356057-34-6	666.79	NA	Solid	Pharmaceutical Substances	

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow ¹	Physical Form	Chemical Class ²	Structure ³
1,4-Dihydroquinone	Hydroquinone; p-hydroquinone	123-31-9	110.11	1.03	Solid	Phenols	
2,4-Dinitrobenzene sulfonic acid	DNBS	89-02-1	248.17	-1.53	Solid	Hydrocarbons, Cyclic; Sulfur Compounds	
Dinocap EC	Butenoic acid, 2-(or 4)-isooctyl-4,6(or 2,6)-dinitrophenyl ester(9CI)Crotonic acid, 2(or 4)-(1-methylheptyl)-4,6(or 2,6)-dinitrophenylester	39300-45-3	366.41	5.98	Liquid	Nitro Compounds; Hydrocarbons, Cyclic	
Formaldehyde	Formalin	50-00-0	30.03	0.35	Liquid	Aldehydes	

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow ¹	Physical Form	Chemical Class ²	Structure ³
Glutaraldehyde	Glutaral; Pentanedial	111-30-8	100.12	-0.18	Liquid	Aldehydes	
Hexyl cinnamic aldehyde	HCA; alpha-Hexylcinnamic aldehyde; alpha-Hexyl cinnamaldehyde	101-86-0	216.33	4.82	Liquid	Aldehydes	
Methyl 4-hydroxybenzoate	Methylparaben	99-76-3	152.15	2	Solid	Carboxylic Acids; Phenols	
Methyl 2-nonynoate	2-Nonynoic acid methyl ester	111-80-8	168.23	3.1	Liquid	Lipids	
Neomycin sulfate	NA	1405-10-3	712.72	NA	Solid	Carbohydrates	

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow ¹	Physical Form	Chemical Class ²	Structure ³
Oxyfluorfen EC	NA	42874-03-3	361.7	5.21	Solid	Ethers	
Pluronic L92	NA	NA	NA	NA	Liquid	NA	NA
Propylene glycol	1,2-Dihydroxypropane; 1,2-Propanediol	57-55-6	76.09	0.43	Liquid	Alcohols	
Quinoxifen SC	NA	124495-18-7	308.13	5.69	Liquid	Heterocyclic Compounds	
Saturated diglycerin	NA	NA	NA	NA	Liquid	Alcohols; Ethers	NA

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow ¹	Physical Form	Chemical Class ²	Structure ³
Sodium lauryl sulfate	Sodium dodecyl sulfate; SLS; SDS; Irium	151-21-3	288.38	1.69	Solid	Alcohols; Sulfur Compounds; Lipids	
Sodium metasilicate	NA	6834-92-0	122.06	-5.65	Solid	Minerals; Silicon Compounds	
Trifluralin EC	NA	1582-09-8	335.28	5.31	Solid	Hydrocarbons, Cyclic; Amines	

Abbreviations: CASRN=Chemical Abstract Services Registry Number; g/mol=Grams per mole; Kow=Octanol-water partition coefficient; NA=Not available.

¹Kow represents the octanol-water partition coefficient (expressed on log scale) obtained from the website: http://www.syrres.com/esc/est_kowdemo.htm.

²Chemical classifications based on the Medical Subject Headings classification for chemicals and drugs, as developed by the National Library of Medicine at: <http://www.nlm.nih.gov/mesh/meshhome.html>. Chemical classification of "pharmaceutical substances" for the GSK chemicals was suggested by Dr. Michael Olson of GSK, which captures three types of pharmaceutical active substances (actives, intermediates, and starting materials).

³Chemical structures, based on CASRN, were obtained from ChemID available at: <http://chem.sis.nlm.gov/chemidplus/chemidheavy.jsp>.