

Supplemental Table 1. Physicochemical properties, % recovery in the volatility test and mass balance of the chemicals tested. The dose and solvent used in the skin penetration and volatility assays are also listed. Physicochemical properties for all chemicals used in the

Volatility pre-test: % recovery at RT, apart from selected chemicals which were incubated at 32°C (denoted in red font))

Chemical	CAS number	Physicochemical properties used in calculations						Volatility pre-test	Skin penetration assay			
		MP (°C)	BP (°C)	Solubility (mg/ml)	LogP	Volatility			% recovery (at 32°C)	Mass Balance		Dose applied (ug/cm ²)
						Henry's law (atm-m ³ /mole)	VP (mmHg)	mean		SD		
1,4-Dihydroquinone (Hydroquinone)	123-31-9	172	286	8.28	0.59	5.50E-08	2.40E-05	95	92.85	3.86	15.73	0.01M PBS
1,4-Phenylenediamine	106-50-3	142	268	0.78	-0.3	5.85E-08	2.78E-03	82	81.75	6.63	0.91	0.01M PBS
2,4-Dichloroacetophenone	937-20-2	101	270	0.04	2.27	1.13E-06	2.33E-02	28	25.59	4.1	0.78	0.01M PBS
2,4-Dinitrochlorobenzene	97-00-7	50.8	315	3.18	2.17	2.46E-07	8.49E-05	76	74.56	14.56	4.26	0.1M PBS
2,5-Diaminotoluene sulfate	615-50-9	83.7	269	59.32	0.2	5.91E-08	2.23E-03	ND	94.3	2.9	0.94	0.01M PBS+AOS
2-Acetyl aminofluorene	53-96-3	193	303	0.97	3.12	1.56E-10	1.98E-08	115	94.9	1.95	1.3	100% ethanol
2-amino-3-methylimidazo[4,5-f]quinoline	76180-96-6	300	379	1.40	1.47	5.38E-08	7.23E-06	98	98.61	1.76	3.21	0.01M PBS
2-Nitro-1,4-phenylenediamine	5307-14-2	138	331	0.60	0.53	1.08E-07	1.32E-05	96	98.75	2.26	5.78	0.01M PBS
4-Amino-3-nitrophenol	610-81-1	151	324	0.35	0.41	4.08E-08	1.42E-06	99	97.2	2.19	11.76	0.01M PBS
4-Aminophenol	123-30-8	188	261	0.96	0.04	9.00E-08	4.00E-05	69	94.94	2.62	4.48	0.01M PBS+AOS
4-Bromophenyl isocyanate	2493-02-9	31.3	226	2.13	3.48	4.84E-07	8.15E-02	117	92.24	6.89	1.24	Ethanol
4-Chloroaniline	106-47-8	70.7	232	17.50	1.83	3.38E-07	2.70E-02	82	59	7.41	5.08	0.01M PBS
4-Chlorobutyric acid	627-00-9	16	229	8.09	1.32	6.61E-07	4.88E-02	50	98.53	1.5	66.36	0.1M PBS
4-Methylvaleric acid	646-07-1	-33	201	7.90	1.98	8.00E-07	1.41E-01	20	37.66	7.47	20.3	0.1M PBS
4-Nitro-o-Phenylenediamine	99-56-9	200	421	0.21	0.88	5.66E-09	1.69E-06	ND	96.32	2.47	1.18	0.01M PBS
4-Tolunitrile	104-85-8	28.1	217	1.27	2.09	2.86E-05	3.13E-01	19	19.6	3.27	1.89	0.01M PBS
6-Methylcoumarin	92-48-8	75.7	303	0.79	1.91	4.43E-08	5.88E-04	ND	99.84	2.3	4.21	0.01M PBS
7-Ethoxycoumarin	31005-02-4	90.1	318	9.05	2.3	3.95E-09	1.76E-04	ND	97.24	3.18	1.13	0.01M PBS
Acetophenone	98-86-2	19.6	202	1.99	1.58	1.04E-05	3.97E-01	7	15.9	7	10.27	0.1M PBS
Basic Red 76 (Chloride salt)	68391-30-0	192	329	2.34	-0.32	8.25E-08	5.48E-10	ND	97.37	1.54	53.27	0.01M PBS
Benzoic Acid	65-85-0	123	249	3.98	1.87	2.62E-07	7.00E-04	ND	91.41	2.25	7.92	0.01M PBS
Benzophenone	119-61-9	48.3	305	8.86	3.18	1.10E-06	1.93E-03	100	73.16	7.3	1.28	0.01M PBS
Benzyl bromide	100-39-0	-3.13	199	0.52	2.92	2.35E-03	4.50E-01	14	6.44	2.87	9.12	100% acetone
Benzylidene acetone	122-57-6	41.8	262	4.45	2.07	1.60E-06	1.24E-02	60	80.27	2.4	3.91	0.01M PBS
Caffeine	58-08-2	236	337	0.00	-0.07	1.59E-06	1.22E-06	ND	97.11	2.21	1.08	0.01M PBS
Cinnamic acid	140-10-3	134	224	0.22	2.13	3.09E-08	1.49E-03	103	98.66	1.44	1.62	0.1M PBS
Cinnamyl Alcohol	104-54-1	33.3	255	3.25	1.95	4.69E-07	2.40E-02	ND	91.49	4.02	6.72	0.01M PBS
Cyclophosphamide monohydrate	6055-19-2	41	325	0.53	0.63	1.36E-11	1.24E-04	ND	96.88	2.12	47.42	0.1M PBS
Diethyleneglycol butyl ether	112-34-5	-68	231	7.32	0.56	7.20E-09	2.19E-02	2	13.19	8.64	64.11	0.1M PBS
Diethylmaleate	141-05-9	-6.83	221	471.60	2.2	2.69E-06	1.05E-01	19	41.75	12.52	24.08	7.3
Dimethyl phthalate	131-11-3	4.44	284	8.46	1.6	9.36E-08	3.08E-03	77	78.95	7.46	1.31	0.01M PBS
Ethylhexyl acrylate	103-11-7	-90	181	8.48	4.09	2.41E-04	1.78E-01	56	29.66	0.79	6.63	0.01M PBS+AOS
Eugenol	97-53-0	-9.65	254	0.63	2.27	2.17E-07	2.26E-02	71	64.33	16.46	6.23	0.1M PBS+AOS
Geraniol	106-24-1	-15	169	503.68	3.56	5.34E-07	3.00E-02	22	34.34	8.33	2.36	0.01M PBS
HC Red No.3	2871-01-4	128	362	0.04	0.51	9.06E-08	2.50E-07	ND	96.82	1.44	21.95	0.01M PBS
Hydrocortisone	50-23-7	217	455	3.65	1.61	9.28E-12	1.86E-10	100	98.16	1.75	5.53	0.01M PBS
Ibuprofen	15687-27-1	73.9	157	0.49	3.97	7.83E-08	1.33E-03	99	101.95	6.08	2.51	0.01M PBS
Isoeugenol	97-54-1	11.8	266	4.69	3.04	2.17E-07	1.20E-02	81	87.25	6.26	3.52	0.1M PBS+AOS
Methyl Methane sulfonate	66-27-3	20	203	0.79	-0.5	2.58E-04	4.14E-01	11	14.15	4.53	24.83	0.1M PBS
Methyl paraben	99-76-3	128	278	530.50	1.96	6.45E-10	4.56E-03	ND	94.24	1.75	3.21	0.01M PBS
Naphthalene	91-20-3	80.3	218	0.12	3.3	4.40E-04	8.50E-02	35	27.3	10.08	0.93	100% ethanol
Nitrobenzene PBS	98-95-3	5.49	211	82.19	1.85	2.40E-05	2.45E-01	11	33.13	4.81	3.7	0.01M PBS
Propyl Paraben	94-13-3	97	283	0.13	3.04	5.71E-10	1.82E-03	101	97.1	6.97	2.51	0.01M PBS
Resorcinol	108-46-3	111	280	3.21	0.8	5.46E-08	4.89E-04	ND	96.5	2.5	97.86	0.01M PBS
Testosterone	58-22-0	138	160	15.45	3.32	2.46E-08	2.10E-07	100	94.83	6.06	1.64	100% ethanol
Tetramethyl thiuram disulfide	137-26-8	154	129	0.41	1.73	2.01E-09	1.73E-05	98	83.87	4.01	1.21	Ethanol
Thioglycolic acid	68-11-1	-15.1	187	0.03	0.09	8.59E-09	8.68E-02	77	85.93	3.4	72.46	0.1M PBS
trans-Cinnamaldehyde	14371-10-9	-7.55	249	0.41	1.9	9.37E-05	3.84E-02	43	61.3	7.41	2.42	0.1M PBS
Triclosan	3380-34-5	48	352	0.76	4.76	6.29E-10	1.14E-05	72	94.28	1.89	1.81	100% Ethanol
Vanillin	121-33-5	82.1	285	495.34	1.21	2.81E-09	1.18E-04	86	81.76	4.08	3.3	0.01M PBS