

Annex III

Traditional LLNA Data Used for the Performance Analysis of the rLLNA

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Substance Name	CASRN	Vehicle	rLLNA ¹	Trad. LLNA ¹	EC3 ²	1 Conc. (%)	1 SI	2 Conc. (%)	2 SI	3 Conc. (%)	3 SI	4 Conc. (%)	4 SI	5 Conc. (%)	5 SI	6 Conc. (%)	6 SI	Data Source
Resorcinol	108-46-3	AOO	+	+	6	1	1.80	2.5	2.30	5.0	2.60	10	6.30	25	10.10	50	12.50	Basketter et al. (2007)
A SC600		PA/H ₂ O	-	-	NC	10	1.40	25	1.80	50	2.30	100	1.60					Bayer CropScience SA Studies, Submitted by E. Debruyne
AE F016382 00 TK71 A101		PA/H ₂ O	-	-	NC	3.6	1.00	7.1	0.80	17.9	1.00	35.7	1.10					Bayer CropScience SA Studies, Submitted by E. Debruyne
D EC25\		PA/H ₂ O	-	-	NC	0.5	0.56	1	0.63	2.5	0.59							Bayer CropScience SA Studies, Submitted by E. Debruyne
D EW 15		PA/H ₂ O	-	-	NC	2.5	1.90	5	1.50	10	2.50	25	2.50					Bayer CropScience SA Studies, Submitted by E. Debruyne
EXP 10810 A		PA/H ₂ O	+	+	2.1	10	6.40	25	8.40	50	9.20							Bayer CropScience SA Studies, Submitted by E. Debruyne
EXP 11120 A		PA/H ₂ O	+	+	64.9	10	0.96	25	0.66	50	1.60	100	6.30					Bayer CropScience SA Studies, Submitted by E. Debruyne
F & Fo WG 50 + 25		PA/H ₂ O	+	+	0.003 1	2.5	11.70	5	12.60	10	14.10	25	15.20					Bayer CropScience SA Studies, Submitted by E. Debruyne
FAR01042-00		PA/H ₂ O	-	-	NC	10	1.40	25	2.10	50	1.40	100	2.50					Bayer CropScience SA Studies, Submitted by E. Debruyne
FAR01060-00		PA/H ₂ O	+	+	88.5	10	0.40	25	0.80	50	1.00	100	3.60					Bayer CropScience SA Studies, Submitted by E. Debruyne
Fx + Me EW 69		PA/H ₂ O	+	+	25.2	5	0.83	10	1.55	25	2.95	50	8.55					Bayer CropScience SA Studies, Submitted by E. Debruyne
1-(2,3-epoxypropoxy)-2,2-bis [(2,3-epoxypropoxy)-methylbutane		ACE	+	+	1.4	1	2.06	3	6.52	10	12.00							BGIA Study Report, Submitted by H.W. Vohr
1,2-Diaminocyclohexane	1436-59-5	ACE	+	+	0.4	0.1	1.19	0.3	1.81	1	8.39							BGIA Study Report, Submitted by H.W. Vohr

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1,6-Bis(2,3-epoxypropoxy)-hexane	16096-31-4	ACE	+	+	1.9	0.3	0.94	1	1.67	3	4.65							BGIA Study Report, Submitted by H.W. Vohr
3-Aminomethyl-3,5,5-trimethylcyclohexyl amine	2855-13-2	ACE	+	+	1.0	0.3	1.17	1	2.68	3	20.16							BGIA Study Report, Submitted by H.W. Vohr
Bakelite EPR 161	9012-45-7	ACE	+	+	0.7	0.1	1.02	0.3	2.37	1	3.49							BGIA Study Report, Submitted by H.W. Vohr
Bakelite EPR 162	9012-45-7	ACE	+	+	0.1	0.3	10.53	1	19.94	3	39.89							BGIA Study Report, Submitted by H.W. Vohr
Bakelite EPR 164	9012-45-7	ACE	+	+	0.2	0.3	5.58	1	16.11	3	28.13							BGIA Study Report, Submitted by H.W. Vohr
Dipropylene triamine	56-18-8	ACE	+	+	0.9	0.3	2.16	1	3.17	3	12.45							BGIA Study Report, Submitted by H.W. Vohr
Hexyl cinnamic aldehyde	101-86-0	AOO	-	-	NC	2.5	1.12	5	1.19	10	2.84							BGIA Study Report, Submitted by H.W. Vohr
Hexyl cinnamic aldehyde	101-86-0	ACE	+	+	1.2	3	4.56	10	6.63	30	9.86							BGIA Study Report, Submitted by H.W. Vohr
Hydroxyethyl-ethylenediamine	111-41-1	ACE	+	+	IDR ³	3	2.00	10	1.72	30	6.60							BGIA Study Report, Submitted by H.W. Vohr
m-Phenylenebis-(methylamine)	1477-55-0	ACE	+	+	0.4	0.3	1.92	1	9.09	3	44.20							BGIA Study Report, Submitted by H.W. Vohr
Oxirane, mono((C12-14-alkyloxy)methyl) derivs	68609-97-2	ACE	+	+	0.6	0.3	2.35	1	4.16	3	22.74							BGIA Study Report, Submitted by H.W. Vohr
p-tert-Butylphenyl-glycidylether	3101-60-8	ACE	+	+	0.4	0.1	1.36	0.3	1.68	1	14.22							BGIA Study Report, Submitted by H.W. Vohr
Sodium lauryl sulfate	151-21-3	Pluronic L92	+	+	4.9	5	3.05	10	4.78	25	8.46							BGIA Study Report, Submitted by H.W. Vohr
Trimethylhexamine diamine		ACE	+	+	1.9	1	2.15	3	4.00	10	8.86							BGIA Study Report, Submitted by H.W. Vohr
Benzalkonium chloride	8001-54-5	ACE	+	+	0.1	0.5	9.00	1	11.10	2	7.60							CESIO Report, Submitted by K. Skirda

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Fatty acid glutamate			+	+	IDR ³	5	1.50	25	1.80	50	1.20	100	4.80					CESIO Report, Submitted by K. Skirda
Glyceryl thioglycolate	30618-84-9	AOO	+	+	4.7	10	8.00	25	14.00	50	31.00							CESIO Report, Submitted by K. Skirda
Laurylglycerin derivative		DMF	+	+	24.3	5	1.62	10	2.36	25	3.03							CESIO Report, Submitted by K. Skirda
Non-ionic surfactant 1		AOO	+	+	27.5	25	2.80	50	4.80	100	6.50							CESIO Report, Submitted by K. Skirda
Non-ionic surfactant 2		AOO	-	+	47.1	25	1.50	50	3.20	100	2.90							CESIO Report, Submitted by K. Skirda
Non-ionic surfactant 3		AOO	+	+	19.8	25	4.70	50	9.80	100	13.30							CESIO Report, Submitted by K. Skirda
Non-ionic surfactant 4		AOO	+	+	0.012	25	36.00	50	39.00	100	162.00							CESIO Report, Submitted by K. Skirda
Non-ionic surfactant 5		AOO	+	+	37.5	25	2.70	50	3.30	100	3.20							CESIO Report, Submitted by K. Skirda
Non-ionic surfactant 6		AOO	+	+	34.4	25	2.70	50	3.50	100	6.50							CESIO Report, Submitted by K. Skirda
Non-ionic surfactant 7		AOO	+	+	IDR ³	25	6.30	50	50.80	100	7.40							CESIO Report, Submitted by K. Skirda
Non-ionic surfactant 8		AOO	+	+	IDR ³	25	4.20	50	3.30	100	5.60							CESIO Report, Submitted by K. Skirda
Non-ionic surfactant 9		AOO	+	+	10.5	25	3.50	50	3.90	100	7.70							CESIO Report, Submitted by K. Skirda
Precursor surfactant 1		AOO	+	+	60.7	25	2.20	50	2.70	100	4.10							CESIO Report, Submitted by K. Skirda
Precursor surfactant 2		AOO	+	+	24.0	25	3.10	50	4.80	100	4.40							CESIO Report, Submitted by K. Skirda
Saturated diglycerin		EtOH/H ₂ O	-	-	NC	25	1.40	50	2.10	100	1.90							CESIO Report, Submitted by K. Skirda
Unsaturated fatty acid		AOO	+	+	22.2	25	3.40	50	5.70	100	6.50							CESIO Report, Submitted by K. Skirda

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Unsaturated fatty acid ester		AOO	+	+	27.1	25	2.80	50	5.20	100	4.70							CESIO Report, Submitted by K. Skirda
Atrazine SC	1912-24-9	Pluronic L92 (1%)	+	+	31.3	12.5	1.80	25	2.80	50	3.60	75	7.10	100	7.30			ECPA LLNA Project Report, Submitted by P. Botham
Dinocap EC	39300-45-3	Pluronic L92 (1%)	+	+	1.1	0.8	2.00	4	14.20	21	26.70							ECPA LLNA Project Report, Submitted by P. Botham
Oxyfluorfen EC	42874-03-3	Pluronic L92 (1%)	-	-	NC	1	0.30	7	0.90	33	2.30							ECPA LLNA Project Report, Submitted by P. Botham
Quinoxifen SC	124495-18-7	Pluronic L92 (1%)	-	-	NC	7	1.10	33	1.70	100	0.80							ECPA LLNA Project Report, Submitted by P. Botham
Quinoxifen/cyproconazole	124495-18-7/ 113096-99-4	Pluronic L92 (1%)	+	+	27.8	12.5	2.00	25	2.30	50	8.60	75	15.80	100	30.10			ECPA LLNA Project Report, Submitted by P. Botham
Trifluralin EC	1582-09-8	Pluronic L92 (1%)	+	+	7.0	7	3.10	33	26.30	100	61.50							ECPA LLNA Project Report, Submitted by P. Botham
Fumaric acid	110-17-8	DMSO	-	-	NC	5	1.30	10	2.30	25	1.40							EFfCI study, Submitted by P. Ungeheuer
Linoleic acid	60-33-3	AOO	+	+	14.1	10	1.50	25	7.00	50	9.10							EFfCI study, Submitted by P. Ungeheuer
Linolenic acid	463-40-1	AOO	+	+	9.9	10	3.10	25	9.30	50	10.30							EFfCI study, Submitted by P. Ungeheuer
Maleic acid	110-16-7	DMSO	+	+	7.0	10	6.70	25	16.10	50	16.10							EFfCI study, Submitted by P. Ungeheuer
Octinol	111-87-5	AOO	+	+	4.7	10	5.60	25	8.80	50	11.20							EFfCI study, Submitted by P. Ungeheuer
Oleic acid	112-80-1	AOO	+	+	10.5	10	2.60	25	14.90	50	6.90							EFfCI study, Submitted by P. Ungeheuer
Squalene	111-02-4	AOO	+	+	7.9	10	3.80	25	6.90	50	8.20							EFfCI study, Submitted by P. Ungeheuer

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Succinic acid	110-15-6	DMSO	-	-	NC	5	1.20	10	1.20	25	1.30							EFfCI study, Submitted by P. Ungeheuer
Undecylenic acid	112-38-9	AOO	+	+	19.4	10	2.50	25	3.30	50	4.40							EFfCI study, Submitted by P. Ungeheuer
1-(2',3',4',5'-Tetramethylphenyl)-3-(4'-tetrabutylphenyl)-propane-1,3-dione		ACE	-	-	NC	10	1.60	20	1.20	40	1.60							Gerberick et al. (2005)
1-(2',3',4',5'-Tetramethylphenyl)butane-1,3-dione	167998-73-4	ACE	+	+	8.3	10	7.00	20	22.10	40	22.40							Gerberick et al. (2005)
1-(2',5'-Dimethylphenyl)butane-1,3-dione	56290-55-2	ACE	+	+	12.5	10	2.3	20	5.1	40	9.5							Gerberick et al. (2005)
1-(2',5'-diethylphenyl)butane-1,3-dione	167998-76-7	ACE	+	+	9.6	10	3.9	20	19.2	40	18.7							Gerberick et al. (2005)
1-(3',4',5'-Tetramethoxyphenyl)-4-dimethylpentane-1,3-dione	135099-98-8	ACE	-	-	NC	10	2.80	20	1.10	40	0.70							Gerberick et al. (2005)
1-(p-methoxyphenyl)-1-penten-3-one	104-27-8	AOO	+	+	9.3	10	3.5	25	10	50	26.1							Gerberick et al. (2005)
1,1,3-Trimethyl-2-formylcyclohexa-2,4-dione	116-26-7	AOO	+	+	7.5	0.5	0.70	1	1.10	2.5	1.10	5	2.70	10	3.30			Gerberick et al. (2005)
1,2-Benzisothiazolin-3-one	2634-33-5	DMF	+	+	2.3	10	3.80	30	4.40	50	4.90							Gerberick et al. (2005)
1,2-Dibromo-2,4-dicyanobutane	35691-65-7	AOO	+	+	0.9	0.5	1.40	1	3.40	2.5	3.50	5	5.40					Gerberick et al. (2005)
1,4-dihydroquinone	123-31-9	AOO	+	+	0.1	0.1	2.80	0.25	5.80	0.5	13.70	1	15.20	2.5	13.10			Gerberick et al. (2005)
12-Bromo-1-dodecanol	3344-77-2	AOO	+	+	6.9	5	2.20	10	4.3	25	9.8							Gerberick et al. (2005)
12-Bromododecanoic acid	73367-80-3	AOO	+	+	17.9	5	1.30	10	2.00	25	3.9							Gerberick et al. (2005)
1-Bromobutane	109-65-9	AOO	-	-	NC	5	1.1	10	1.2	25	1							Gerberick et al. (2005)
1-Bromodocosane	6938-66-5	AOO	+	+	8.3	2.5	1.2	5	1.6	10	3.7							Gerberick et al. (2005)
1-Bromododecane	143-15-7	AOO	+	+	17.7	5	1.1	10	1.4	25	4.5							Gerberick et al. (2005)

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1-Bromoeicosane	4276-49-7	AOO	+	+	6.1	5	2.1	10	6.2	25	8.4							Gerberick et al. (2005)
1-Bromoheptadecane	3508-00-7	AOO	+	+	4.8	5	3.2	10	6	25	9.6							Gerberick et al. (2005)
1-Bromohexadecane	112-82-3	AOO	+	+	2.3	1	1.1	2.5	3.3	5	7.9	10	11.1	25	13.5	50	16.8	Gerberick et al. (2005)
1-Bromohexane	111-25-1	AOO	+	+	10.3	1	1.7	10	2.9	50	18.6							Gerberick et al. (2005)
1-Bromononane	693-58-3	AOO	-	-	NC	5	1.2	10	1.4	25	2.8							Gerberick et al. (2005)
1-Bromooctadecane	112-89-0	AOO	+	+	15.2	5	1.8	10	2.2	25	4.5							Gerberick et al. (2005)
1-Bromopentadecane	629-72-1	AOO	+	+	5.1	5	2.9	10	7.8	25	19.6							Gerberick et al. (2005)
1-Bromotetradecane	112-71-0	AOO	+	+	9.2	5	1.5	10	3.3	25	11.3							Gerberick et al. (2005)
1-Bromotridecane	765-09-3	AOO	+	+	10.2	5	1.6	10	2.9	25	10.4							Gerberick et al. (2005)
1-Bromoundecane	693-67-4	AOO	+	+	19.6	5	1.3	10	1.4	25	3.9							Gerberick et al. (2005)
1-Butanol	71-36-3	dH ₂ O	-	-	NC	5	1.6	10	1.2	20	1.4							Gerberick et al. (2005)
1-Chloro-2,4-dinitrobenzene	97-00-7	AOO	+	+	0.05	0.01	1.50	0.025	1.8	0.05	2.4	0.1	8.9	0.25	38			Gerberick et al. (2005)
1-Chlorohexadecane	4860-03-1	AOO	+	+	9.1	5	1.6	10	3.3	25	5.7							Gerberick et al. (2005)
1-Chloromethylpyrene	1086-00-6	AOO	+	+	0.005	0.025	11.6	0.05	15.4	0.1	18.6							Gerberick et al. (2005)
1-Chlorononane	2473-01-0	AOO	-	-	NC	10	1	25	1.6	50	2.3							Gerberick et al. (2005)
1-Chlorooctadecane	3386-33-2	AOO	+	+	16.3	10	1.7	25	4.8	50	7.3							Gerberick et al. (2005)
1-Chlorotetradecane	2425-54-9	AOO	+	+	20.2	10	1.1	25	3.9	50	6.3							Gerberick et al. (2005)
1-Iododecane	4292-19-7	AOO	+	+	13.1	5	1.70	10	2.30	25	5.70							Gerberick et al. (2005)
1-Iodoheptadecane	544-77-4	AOO	+	+	19.1	10	1.60	25	3.90	50	6.40							Gerberick et al. (2005)
1-Iodoheptane	638-45-9	AOO	-	-	NC	10	0.90	25	1.20	50	2.50							Gerberick et al. (2005)
1-Iodononane	4282-42-2	AOO	+	+	24.2	10	1.30	25	3.10	50	4.60							Gerberick et al. (2005)
1-Iodoctadecane	629-93-6	AOO	-	-	NC	5	1	10	1.4	25	1.9							Gerberick et al. (2005)
1-Iodotetradecane	19218-94-1	AOO	+	+	13.8	10	1.70	25	6.90	50	9.70							Gerberick et al. (2005)
1-Methyl-3-nitro-nitrosoguanidine	70-25-7	AOO	+	+	0.03	0.05	27.5	0.1	60.4	0.25	78.3							Gerberick et al. (2005)

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1-Naphthol	90-15-3	AOO	+	+	1.3	0.1	1.40	0.25	1.00	0.5	1.20	1	1.50	2.5	8.50			Gerberick et al. (2005)
1-Phenyl-1,2-propanedione	579-07-7	AOO	+	+	1.3	5	12.80	10	17.70	25	20.10							Gerberick et al. (2005)
1-Phenyl-2-methylbutane-1,3-dione	6668-24-2	ACE	+	+	29.1	10	1.70	20	2.00	40	4.20							Gerberick et al. (2005)
1-Phenyloctane-1,3-dione	55846-68-1	ACE	+	+	10.4	10	2.80	20	6.60	40	8.70							Gerberick et al. (2005)
2-(4-Amino-2nitrophenylamino)-ethanol	2871-01-4	AOO	+	+	2.2	0.1	0.50	0.25	1.20	0.5	1.90	1	1.8	2.5	3.3			Gerberick et al. (2005)
2-(4-tert-Amylcyclohexyl) acetaldehyde	620159-84-4	AOO	+	+	36.8	25	2.1	50	4.00	100	9.10							Gerberick et al. (2005)
2,2,6,6-Tetramethylheptane-3,5-dione	1118-71-4	ACE	+	+	26.7	10	2.10	20	2.80	40	3.40							Gerberick et al. (2005)
2,3-Butanedione	431-03-8	AOO	+	+	11.3	5	1.4	10	2.8	25	5.2							Gerberick et al. (2005)
2,4,6-Trichloro-1,3,5-triazine	108-77-0	AOO	+	+	0.09	1	21.80	2.5	28.90	5	34.00							Gerberick et al. (2005)
2,4-Heptadienal	5910-85-0	AOO	+	+	4.0	0.5	1.1	1	1.4	2.5	1.9	5	3.7	10	8.10			Gerberick et al. (2005)
2,5-Diaminotoluene	95-70-5	DMSO	+	+	0.17	0.125	2.6	0.25	3.5	0.5	4.1	1	5.5					Gerberick et al. (2005)
2-Acetylcyclohexanone	874-23-7	ACE	-	-	NC	10	0.8	20	0.7	40	0.8							Gerberick et al. (2005)
2-Amino-6-chloro-4-nitrophenol	6358-09-4	AOO	+	+	2.2	0.1	1.7	0.25	1.4	0.5	2.1	1	1.5	2.5	3.4			Gerberick et al. (2005)
2-Aminophenol	95-55-6	AOO	+	+	0.4	0.5	3.5	1	5	2.5	7.4							Gerberick et al. (2005)
2-Bromotetradecanoic acid	10520-81-7	AOO	+	+	3.4	5	4.7	10	7.7	25	10.1							Gerberick et al. (2005)
2-Hydroxyethyl acrylate	818-61-1	AOO	+	+	1.4	5	10.70	10	14.80	25	18.10							Gerberick et al. (2005)
2-Hydroxypropyl methacrylate	923-26-2	AOO	-	-	NC	10	1.1	25	1.2	50	1.3							Gerberick et al. (2005)
2-Mercapto-benzothiazole	149-30-4	DMF	+	+	1.7	1	2.3	3	4.4	10	8.6							Gerberick et al. (2005)
2-Methoxy-4-methylphenol	93-51-6	AOO	+	+	5.8	4.2	1.80	8.4	5.00	21	8.50							Gerberick et al. (2005)
2-Methyl-2H-isothiazol-3-one	2682-20-4	AOO	-	+	1.9	0.25	1.50	0.5	1.50	1	1.8	2.5	3.8	5	2.5			Gerberick et al. (2005)
2-Methyl-4H,3,1-benzoxazin-4-one	525-76-8	DMSO	+	+	0.7	5	7.60	10	9.20	25	10.80							Gerberick et al. (2005)

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2-Methyl-5-hydroxy-ethylaminophenol	55302-96-0	AOO	+	+	0.4	0.1	1.20	0.25	0.80	0.5	3.60	1	2.6	2.5	7.4			Gerberick et al. (2005)
2-Methylundecanal	110-41-8	AOO	+	+	10.0	0.5	1.40	1	1.30	2.5	1.30	5	2.40	10	3.00			Gerberick et al. (2005)
2-Nitro-p-phenylenediamine	5307-14-2	AOO	+	+	0.4	0.1	1.80	0.25	2.20	0.5	3.30	1	7.90	2.5	11.90			Gerberick et al. (2005)
3 and 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexane-1-carboxaldehyde	31906-04-4	AOO	+	+	17.1	1	0.60	2.5	0.70	5	0.60	10	1.30	25	4.90			Gerberick et al. (2005)
3, 3', 4', 5-Tetrachloro-salicylanilide	1154-59-2	ACE	+	+	0.04	0.25	11.20	0.5	14.40	1	18.00							Gerberick et al. (2005)
3,4-Dihydrocoumarin	119-84-6	AOO	+	+	5.6	2.5	1.6	5	2.5	10	6.6							Gerberick et al. (2005)
3,5,5-Trimethylhexanoyl chloride	36727-29-4	AOO	+	+	2.7	5	7.20	10	12.00	25	19.00							Gerberick et al. (2005)
3-Aminophenol	591-27-5	AOO	+	+	3.2	2.5	2.8	5	3.5	10	5.7							Gerberick et al. (2005)
3-Bromomethyl-5,5'-dimethyl-dihydro-2(3H)-furanone	154750-20-6	AOO	+	+	3.5	3.19	2.7	6.37	5.1	12.74	7.1							Gerberick et al. (2005)
3-Dimethylamino-propylamine	109-55-7	AOO	+	+	2.2	0.5	1.30	1	1.10	2.5	3.50	5	7.00	10	13.90			Gerberick et al. (2005)
3-Ethoxy-1-(2',3',4',5'-tetramethylphenyl)propane-1,3-dione	170928-69-5	ACE	+	+	33	10	1.1	20	1.7	40	3.7							Gerberick et al. (2005)
3-Methyl-4-phenyl-1,2,5-thiadiazole-1,1-dioxide	3775-21-1	AOO	+	+	1.4	0.1	1.3	0.25	1.1	0.5	2.1	1	1.9	2.5	5.6			Gerberick et al. (2005)
3-Methyleugenol	186743-26-0	AOO	+	+	32	11	1.5	27	2.3	54	6.4							Gerberick et al. (2005)
3-Methylisoeugenol	186743-29-3	AOO	+	+	3.6	2.5	2.20	5.5	4.30	11	6.00							Gerberick et al. (2005)
3-Phenylene-diamine	108-45-2	AOO	+	+	0.5	2.5	11.70	5	15.50	10	19.20							Gerberick et al. (2005)
3-Propyliden-phthalide	17369-59-4	AOO	+	+	3.7	5	4.90	10	9.10	25	15.10							Gerberick et al. (2005)
4-(N-Ethyl-N-2-methan-sulfamido-ethyl)-2-methyl-1,4-phenylene-diamine	25646-71-3	DMSO	+	+	0.6	0.1	1.2	1	4.5	5	5.9	10	6.3					Gerberick et al. (2005)

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4,4,4-Trifluoro-1-phenylbutane-1,3-dione	362-06-7	ACE	+	+	20	10	2.10	20	3.00	40	4.60							Gerberick et al. (2005)
4-Allylanisole	140-67-0	AOO	+	+	18	10	1.20	25	4.7	50	4.5	100	8					Gerberick et al. (2005)
4-Hydroxybenzoic acid	99-96-7	DMSO	-	-	NC	5	1.4	10	1.5	25	1.3							Gerberick et al. (2005)
4'-Methoxyacetophenone	100-06-1	AOO	-	-	NC	10	1.3	25	1	50	1							Gerberick et al. (2005)
4-Methylamino-phenol sulfate	55-55-0	DMF	+	+	0.8	0.5	2.50	1	3.40	2.5	6.70							Gerberick et al. (2005)
4-Nitrobenzyl bromide	100-11-8	AOO	+	+	0.05	0.01	0.90	0.03	1.30	0.05	3.50	0.1	11.50					Gerberick et al. (2005)
4-Phenylene-diamine	106-50-3	AOO	+	+	0.16	0.05	1.90	0.1	2.30	0.25	4.00	0.5	5.70	1.0	6.60			Gerberick et al. (2005)
5,5-Dimethyl-3-methylenedihydro-2(3H)-furanone	29043-97-8	AOO	+	+	2.0	2	3	4	7.4	8	9.2							Gerberick et al. (2005)
5-Chloro-2-methyl-4-isothiazolin-3-one	26172-55-4	DMF	+	+	0.009	0.01	3.50	0.03	12.30	0.1	22.70							Gerberick et al. (2005)
5-Methyl-2,3-hexanedione	13706-86-0	AOO	+	+	26	25	2.90	50	6.00	100	14.30							Gerberick et al. (2005)
5-Methyleugenol	186743-25-9	AOO	+	+	13	11	2.7	27	4.9	54	4.3							Gerberick et al. (2005)
6-Methylcoumarin	92-48-8	ACE	-	-	NC	5	1	10	1	25	1.1							Gerberick et al. (2005)
6-Methyleugenol	186743-24-8	AOO	+	+	17	11	1.9	27	4.9	54	8.3							Gerberick et al. (2005)
6-Methylisoeugenol	13041-12-8	AOO	+	+	1.6	2.5	5.90	5.5	11.10	11	15.7							Gerberick et al. (2005)
7,12-Dimethyl-benz[a]anthracene	57-97-6	DMF	+	+	0.006	0.025	7.60	0.5	17.70	1	15.60							Gerberick et al. (2005)
7-Bromotetradecane	74036-97-8	AOO	+	+	21	5	0.9	10	1.2	25	3.6							Gerberick et al. (2005)
Abietic acid	514-10-3	AOO	+	+	15	5	1.5	10	2	25	5.2							Gerberick et al. (2005)
alpha-Amyl cinnamic aldehyde	122-40-7	AOO	+	+	10.6	1	1.5	2.5	1.7	5	2.2	10	2.8	25	8.2			Gerberick et al. (2005)
alpha-Butyl cinnamic aldehyde	7492-44-6	AOO	+	+	11.2	1	1.4	2.5	1.7	5	1.7	10	2.1	25	13			Gerberick et al. (2005)
alpha-Methyl cinnamic aldehyde	101-39-3	AOO	+	+	4.5	1	1.80	2.5	1.50	5	3.40	10	3.3	25	15.3			Gerberick et al. (2005)
alpha-Methylphenyl-acetaldehyde	93-53-8	AOO	+	+	6.3	0.5	2	1	2.2	2.5	1	5	2.2	10	5.2			Gerberick et al. (2005)
Aniline	62-53-3	AOO	+	+	89	5	1.1	10	0.9	25	2	50	1.9	100	3.3			Gerberick et al. (2005)

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Benzaldehyde	100-52-7	AOO	-	-	NC	1	2.1	2.5	1.7	5	2.2	10	1.8	25	2			Gerberick et al. (2005)
Benzene-1,3,4-tricarboxylic anhydride	552-30-7	AOO	+	+	9.2	1	1.10	2.5	2.00	5	2.00	10	3.20	25	4.60			Gerberick et al. (2005)
Benzo[a]pyrene	50-32-8	AOO	+	+	0.0009	0.5	17.6	1	19.2	2.5	27							Gerberick et al. (2005)
Benzocaine	94-09-7	AOO	-	-	NC	2.5	2.1	5	1.8	10	2.7	25	1.8	50	1.2			Gerberick et al. (2005)
Benzoquinone	106-51-4	AOO	+	+	0.0099	0.5	36.4	1	42.3	2.5	52.3							Gerberick et al. (2005)
Benzyl benzoate	120-51-4	AOO	+	+	17	5	2.3	25	3.5									Gerberick et al. (2005)
Benzyl bromide	100-39-0	AOO	+	+	0.2	0.25	3.5	0.5	11.5	1	16.1	2.5	16.4	5	25.1			Gerberick et al. (2005)
Benzylidene acetone	122-57-6	AOO	+	+	3.7	10	8.5	25	13.6	50	12.8							Gerberick et al. (2005)
beta-Propiolactone	57-57-8	AOO	+	+	0.15	0.025	1.50	1.0	13.00	2.5	19.90							Gerberick et al. (2005)
bis-1,3-(2',5'-dimethylphenyl)-propane-1,3-dione		ACE	-	-	NC	10	1.8	20	1.6	40	2.1							Gerberick et al. (2005)
Bisphenol A-diglycidyl ether	1675-54-3	AOO	+	+	1.5	1	2	3	6	10	17.4							Gerberick et al. (2005)
Butyl glycidyl ether	2426-08-6	AOO	+	+	30.9	10	1.40	25	2.20	50	5.60							Gerberick et al. (2005)
C11-azlactone	176665-06-8	AOO	+	+	16	8.3	1.30	20.7	4.00	41.3	8.50							Gerberick et al. (2005)
C15-azlactone	176665-09-1	AOO	+	+	18	10	1.80	25	4.10	50	7.50							Gerberick et al. (2005)
C17-azlactone	176665-11-5	AOO	+	+	19	10.87	1.70	27.17	4.30	54.33	4.60							Gerberick et al. (2005)
C19-azlactone		AOO	-	+	26	11.73	2.50	29.33	3.10	58.67	2.50							Gerberick et al. (2005)
C4-azlactone	176664-99-6	AOO	+	+	1.4	0.52	1.10	1.31	2.30	2.62	4.10	5.23	11.70					Gerberick et al. (2005)
C6-azlactone	176665-02-4	AOO	+	+	1.3	0.61	1.20	1.52	3.50	3.05	7.60							Gerberick et al. (2005)
C9-azlactone	176665-04-6	AOO	+	+	2.8	1.85	1.40	3.7	4.60	7.4	10.10							Gerberick et al. (2005)
Camphorquinone	465-29-2	AOO	-	+	10	5	2.8	10	3	25	1.7							Gerberick et al. (2005)
Chlorobenzene	108-90-7	AOO	-	-	NC	5	1.1	10	1.7	25	1.6							Gerberick et al. (2005)
Cinnamic alcohol	104-54-1	AOO	+	+	21	10	1.8	25	3.5	50	3.9	90	5.7					Gerberick et al. (2005)
Cinnamic aldehyde	104-55-2	AOO	+	+	3.0	0.5	1.40	1.0	0.90	2.5	1.90	5.0	7.10	10.0	15.80			Gerberick et al. (2005)

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cis-6-Nonenal	2277-19-2	AOO	+	+	22	10	1.60	25.0	3.30	50.0	4.50	100.0	13.70					Gerberick et al. (2005)
Citral	5392-40-5	AOO	+	+	13	5	1.20	10	2.10	25	6.30							Gerberick et al. (2005)
Clotrimazole	23593-75-1	AOO	+	+	4.8	2.5	1.6	5	3.1	10	3							Gerberick et al. (2005)
Coumarin	91-64-5	AOO	-	-	NC	5	2.70	10	2.90	25	2.30							Gerberick et al. (2005)
Cyclamen aldehyde	103-95-7	AOO	+	+	22.0	1	1.40	2.5	1.30	10	1.80	25	3.3	50	5.2			Gerberick et al. (2005)
Diethyl maleate	141-05-9	AOO	+	+	5.8	25	16.30	50	22.60	100	13.10							Gerberick et al. (2005)
Diethyl sulfate	64-67-5	AOO	+	+	3.3	1	0.8	2.5	1.9	10	12							Gerberick et al. (2005)
Diethyl-acetaldehyde	97-96-1	AOO	+	+	76	25	1.2	50	0.8	75	2.4	100	16.3					Gerberick et al. (2005)
Diethylenetriamine	111-40-0	AOO	+	+	5.8	10	6.40	25	12.10									Gerberick et al. (2005)
Diethylphthalate	84-66-2	AOO	-	-	NC	25	1.00	50	1.30	100	1.50							Gerberick et al. (2005)
Dihydroeugenol	2785-87-7	AOO	+	+	6.8	5.1	2.70	10.1	3.60	25.3	7.80							Gerberick et al. (2005)
Dimethyl sulfate	77-78-1	AOO	+	+	0.19	0.25	3.80	0.5	6.00	1	5.70							Gerberick et al. (2005)
Dimethyl sulfoxide	67-68-5	AOO	+	+	72	25	2.70	50	2.30	100	3.90							Gerberick et al. (2005)
Dodecyl methanesulfonate	51323-71-8	AOO	+	+	8.8	5	2.10	10	3.30	25	9.00							Gerberick et al. (2005)
Ethyl benzoylacetate	94-02-0	ACE	-	-	NC	10	0.9	20	0.9	40	1.2							Gerberick et al. (2005)
Ethyl vanillin	121-32-4	AOO	-	-	NC	2.5	0.65	5	1.05	10	0.74	25	0.36	50	0.29			Gerberick et al. (2005)
Ethyl acrylate	140-88-5	AOO	+	+	28	10	1.2	25	2.7	50	5							Gerberick et al. (2005)
Ethylene glycol dimethacrylate	97-90-5	MEK	+	+	28	10	1.20	25	2.40	50	7.00							Gerberick et al. (2005)
Ethylenediamine free base	107-15-3	AOO	+	+	2.2	0.1	1.10	0.25	1.20	0.5	1.60	1	1.90	2.5	3.30	5	6.10	Gerberick et al. (2005)
Eugenol	97-53-0	AOO	+	+	13	2.5	1.60	5	1.50	10	2.40	25	5.50					Gerberick et al. (2005)
Farnesal	502-67-0	AOO	+	+	12	1	0.60	2.5	1.10	5	1.70	10	2.50	25	7.00			Gerberick et al. (2005)
Fluorescein isothiocyanate	27072-45-3	ACE/DBP (50:50)	+	+	0.143	0.5	8.60	1	11.70	2.5	16.60							Gerberick et al. (2005)
Formaldehyde	50-00-0	ACE	+	+	0.61	0.093	1.10	0.185	2.30	0.37	2.30	0.925	3.90	1.85	4.00			Gerberick et al. (2005)
Furil	492-94-4	AOO	-	-	NC	5	1.20	10	1.70	25	2.20							Gerberick et al. (2005)

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Geraniol	106-24-1	EtOH/ DEP (75:25)	+	+	26	1	1.00	3	1.00	10	1.30	30	3.40	50	3.90			Gerberick et al. (2005)
Glutaraldehyde	111-30-8	ACE	+	+	0.1	0.05	1.30	0.125	4.30	0.25	7.60	0.5	11.60	1.25	17.70	2.5	18.00	Gerberick et al. (2005)
Glycerol	56-81-5	DMF	-	-	NC	25	1.10	50	0.70	100	0.50							Gerberick et al. (2005)
Glyoxal	107-22-2	AOO	+	+	1.4	1	2.50	2.5	4.20	5	5.20	10	10.30	25	15.80			Gerberick et al. (2005)
Hexane	110-54-3	AOO	-	-	NC	25	0.8	50	0.8	100	2.2							Gerberick et al. (2005)
Hexyl cinnamic aldehyde	101-86-0	AOO	+	+	11	2.5	1.30	5	1.10	10	2.50	25	10.00	50	17.00			Gerberick et al. (2005)
Hydroxycitronellal	107-75-5	AOO	+	+	33	2.5	2.20	5	1.00	10	0.80	25	1.10	50	7.10			Gerberick et al. (2005)
Imidazolidinyl urea	39236-46-9	DMF	+	+	24	10	1.70	25	3.10	50	5.50							Gerberick et al. (2005)
Isoeugenol	97-54-1	AOO	+	+	1.7	0.5	1.00	1	1.10	5	12.40							Gerberick et al. (2005)
Isononanoyl chloride	57077-36-8	AOO	+	+	2.7	5	6.60	10	10.60	25	12.60							Gerberick et al. (2005)
Isopropanol	67-63-0	AOO	-	-	NC	10	1.7	25	1.1	50	1							Gerberick et al. (2005)
Isopropyl myristate	110-27-0	AOO	+	+	44	25	2.10	50	3.30	100	3.40							Gerberick et al. (2005)
Isopropyleugenol	51474-90-9	AOO	-	-	NC	12	1.8	29.0	1.8	59.0	2.2							Gerberick et al. (2005)
Isopropyl-isoeugenol	2953-00-7	AOO	+	+	0.6	0.6	3.00	1.2	5.70	3.0	10.70							Gerberick et al. (2005)
Kanamycin	59-01-8; 8063-07-8	AOO	-	-	NC	5	2.2	10	0.8	25	1							Gerberick et al. (2005)
Lactic acid	598-82-3	DMSO	-	-	NC	5	1	10	1.4	25	2.2							Gerberick et al. (2005)
Lauryl gallate	1166-52-5	DMSO	+	+	0.3	1	12.10	10	29.70	25	29.30	50	36					Gerberick et al. (2005)
Linalool alcohol	78-70-6	AOO	+	+	30	25	2.5	50	4.8	100	8.3							Gerberick et al. (2005)
Methyl dodecanesulfonate	2374-65-4	AOO	+	+	0.4	1	21.6	2.5	39.9	5	48.6							Gerberick et al. (2005)
Methyl hexadecyl sulfonate	4230-15-3	AOO	-	-	NC	5	1	10	1.3	25	1.5							Gerberick et al. (2005)
Methyl hexadecane-sulfonate	26452-48-2	AOO	+	+	0.8	5	26.7	10	35.4	25	32.9							Gerberick et al. (2005)
Methyl methanesulfonate	66-27-3	AOO	+	+	2.7	0.25	0.7	1	0.7	10	3.6							Gerberick et al. (2005)
Methyl salicylate	119-36-8	AOO	-	-	NC	1.0	1	2.5	1.1	5.0	1.6	10	1.4	20	0.9			Gerberick et al. (2005)

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Methyl(2-sulfomethyl) octadecanoate		AOO	+	+	2.0	2.5	5.10	5.0	11.60	10.0	25.60							Gerberick et al. (2005)
Methyl-2-nonynoate	111-80-8	EtOH (80%)	+	+	2.5	5	10.4	10	17.7	20	24.4							Gerberick et al. (2005)
Methyl-4-hydroxybenzoate	99-76-3	DMF	-	-	NC	10	0.80	25	0.90	50	0.80							Gerberick et al. (2005)
N-Ethyl-N-nitrosourea	759-73-9	AOO	+	+	1.1	0.25	1.00	1	2.70	10	22.30							Gerberick et al. (2005)
N-Methyl-N-nitrosourea	684-93-5	AOO	+	+	0.05	0.05	2.7	0.1	7.1	0.25	15.4							Gerberick et al. (2005)
Nonanoyl chloride	764-85-2	AOO	+	+	1.8	5	12.70	10	19.40	25	20.90							Gerberick et al. (2005)
Octanoic acid	124-07-2	AOO	-	-	NC	10	0.70	25.0	1.00	50.0	1.60							Gerberick et al. (2005)
Oleyl methane sulfonate	35709-09-2	AOO	+	+	25	5	1.00	10.0	1.30	25.0	3.00							Gerberick et al. (2005)
Oxalic acid	144-62-7	DMF	+	+	15	5	2.40	10	2.80	25	3.40							Gerberick et al. (2005)
Oxazolone	15646-46-5	AOO	+	+	0.003	0.003	2.90	0.005	4.90	0.01	12.00	0.025	22.00	0.05	33.00			Gerberick et al. (2005)
Palmitoyl chloride	112-67-4	AOO	+	+	8.8	5	2.10	10	3.30	25	4.50							Gerberick et al. (2005)
Penicillin G	61-33-6	DMSO	+	+	30	2.5	1.00	5.0	1.00	10	1.40	25.0	2.10	50.0	6.60			Gerberick et al. (2005)
Pentachlorophenol	87-86-5	DMSO	+	+	20	10	2.10	25.0	3.50	50.0	5.40							Gerberick et al. (2005)
Perillaldehyde	2111-75-3	AOO	+	+	4.0	0.5	1.20	1.0	1.10	2.5	0.90	5.0	4.30					Gerberick et al. (2005)
Phenyl benzoate	93-99-2	AOO	+	+	20	5	2.30	10	2.10	25	3.50							Gerberick et al. (2005)
Phenylacetaldehyde	127-78-1	AOO	+	+	3.0	1	0.70	2.5	1.80	5.0	7.80	10	8.80	25.0	19.00			Gerberick et al. (2005)
p-Methylhydro-cinnamic aldehyde	5406-12-2	AOO	+	+	14	2.5	1.20	5	1.40	10	2.60	25	4.2	50	10.7			Gerberick et al. (2005)
Potassium dichromate	7778-50-9	DMSO	+	+	0.08	0.025	1.60	0.05	1.40	0.1	3.80	0.25	5.30	0.5	16.10			Gerberick et al. (2005)
Propylene glycol	57-55-6	dH ₂ O	-	-	NC	50	1.20	100.0	1.60									Gerberick et al. (2005)
Propylparaben	94-13-3	AOO	-	-	NC	5	1.40	10	1.00	25.0	1.30							Gerberick et al. (2005)
p-tert-Butyl-a-ethyl-hydrocinnamal	80-54-6	AOO	+	+	19	1	1.3	2.5	2.5	10	2	25	3.7	50	9.3			Gerberick et al. (2005)
Pyridine	110-86-1	AOO	+	+	72	25	1.10	50.0	2.30	100.0	3.90							Gerberick et al. (2005)
R(+)-Limonene	5989-27-5	AOO	+	+	69	25	1.8	50	2.4	100	4							Gerberick et al. (2005)

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Saccharin	81-07-2	DMSO	-	-	NC	25	1.30	50.0	1.30	75.0	1.50							Gerberick et al. (2005)
Salicylic acid	69-72-7	AOO	-	-	NC	5	0.80	10	1.50	25.0	2.50							Gerberick et al. (2005)
Sodium lauroyl lactylate	13557-75-0	AOO	+	+	15	5	1.40	10.0	2.50	25.0	3.90							Gerberick et al. (2005)
Sodium lauryl sulfate	151-21-3	DMF	+	+	14	1	0.90	2.5	1.10	5.0	1.70	10.0	2.60	20.0	3.50			Gerberick et al. (2005)
Sodium-3,3,5-trimethyl-hexanoyloxy-benzenesulfonate	94612-91-6	DMSO	+	+	6.4	5	2.30	10.0	4.80	25.0	7.80							Gerberick et al. (2005)
Streptomycin sulfate	3810-74-0	DMF	-	-	NC	2.5	1.20	5.0	1.40	10	1.30	25.0	2.00	50.0	1.90			Gerberick et al. (2005)
Sulfanilamide	63-74-1	DMF	-	-	NC	10.0	1.00	25.0	1.00	50.0	0.90							Gerberick et al. (2005)
Sulfanilic acid	121-57-3	DMF	-	-	NC	5.0	1.50	10	1.90	25.0	2.20							Gerberick et al. (2005)
Tartaric acid	87-69-4	DMF	-	-	NC	5	1.00	10	0.90	25	1.50							Gerberick et al. (2005)
Tetramethyl thiuram disulfide	137-26-8	AOO	+	+	5.2	2.5	2.40	5.0	2.90	10	5.10							Gerberick et al. (2005)
trans-2-Decenal	3913-71-1	AOO	+	+	2.5	0.5	1.30	1	1.10	2.5	3.00	5	6	10	9.5			Gerberick et al. (2005)
trans-2-Hexenal	6728-26-3	AOO	+	+	5.5	0.5	1.2	1	1.2	2.5	2.3	5	2.6	10	6.4			Gerberick et al. (2005)
trans-Anethol	104-46-1	AOO	+	+	2.3	4.5	13.50	9	24.7	22.6	37.3							Gerberick et al. (2005)
Undec-10-enal	112-45-8	AOO	+	+	6.8	5.0	1.70	10	5.30	25.0	7.50	50.0	8.70	75.0	8.80			Gerberick et al. (2005)
Vanillin	121-33-5	AOO	-	-	NC	2.5	0.90	5.0	1.40	10	1.50	25.0	1.20	50.0	1.40			Gerberick et al. (2005)
Vinylidene dichloride	75-35-4	AOO	-	-	NC	10	0.80	25.0	0.80	50.0	0.90							Gerberick et al. (2005)
Vinylpyridine	1337-81-1	AOO	+	+	1.6	2.5	7.40	5.0	14.20	10	14.80							Gerberick et al. (2005)
(16-beta)-21-(Acetyloxy)-17-hydroxy-16-methylpregna-1,4,9(11)-triene-3,20-dione	910-99-6	DMF	-	-	NC	2.5	1.30	5	1.27	10	0.89							Glaxo SmithKline, Submitted by M.J. Olson

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(1r)-1,2,3,4-Tetrahydro-6,7-dimethoxy-2-methyl-1-[(3,4,5-trimethoxyphenyl)methyl]isoquinoline [r-(r*,r*)]-2,3-bis(benzoyloxy)-butanedioate (1:1)	104832-01-1	DMF	-	-	NC	10	0.92	25	1.12	50	1.27							Glaxo SmithKline, Submitted by M.J. Olson
(2-Bromo-5-propoxyphenyl)(2-hydroxy-4-methoxyphenyl)-methadone	190965-45-8	ACE	-	-	NC	0.5	1.10	5	0.90	50	1.70							Glaxo SmithKline, Submitted by M.J. Olson
(2e)-2-[(2-Formyl-4-hydroxyphenyl)-methylidene]-butanedioic acid	773059-57-7	DMF	+	+	48	0.5	0.80	5	1.45	50	3.08							Glaxo SmithKline, Submitted by M.J. Olson
(2-Oxo-1-phenylpyrrolidin-3-yl)(triphenyl)phosphonium bromide	148776-18-5	DMSO	-	-	NC	2.5	1.64	5	2.45	10	1.40							Glaxo SmithKline, Submitted by M.J. Olson
(2R,4S)-4-(4-Acetyl-1-piperazinyl)-n-[(1r)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-n-methyl-1-piperidine-carboxamide monomethanesulfonate	414910-30-8	DMF	-	-	NC	2.5	1.07	5	0.90	10	1.47							Glaxo SmithKline, Submitted by M.J. Olson
(2S,4S)-1-[(2s)-2-Amino-3,3-bis(4-fluorophenyl)-1-oxopropyl]-4-fluoro-2-pyrrolidine carbonitrile	483369-58-0	DMSO	-	-	NC	5	0.99	10	1.60	25	2.44							Glaxo SmithKline, Submitted by M.J. Olson

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(3as,4r,5s,6s,8r,9r,9ar,10r)-6-Ethenyldeca-hydro-5-hydroxy-4,6,9,10-tetramethyl-1-oxo-3a,9-propano-3ah-cyclopentacycloocten-8-yl [[[3-exo)-8-methyl-8-azabicyclo-[3.2.1]oct-3-yl]thio]-acetate	224452-66-8	AOO	-	-	NC	0.5	1.00	2	1.40	5	1.20							Glaxo SmithKline, Submitted by M.J. Olson
(3as,4r,5s,6s,8r,9r,9ar,10r)-6-Ethenyldeca-hydro-5-hydroxy-4,6,9,10-tetra-methyl-1-oxo-3a,9-propano-3ah-cyclopentacycloocten-8-yl hydroxyacetate	125-65-5	DMF	-	-	NC	10	1.38	25	1.42	50	1.56							Glaxo SmithKline, Submitted by M.J. Olson
(3-Endo)-8-methyl-8-azabicyclo[3.2.1]-octan-3-ol	120-29-6	DMF	+	+	8.9	10	4.11	25	12.85	50	26.14							Glaxo SmithKline, Submitted by M.J. Olson
(3r,3as,6ar)-Hexahydrofuro-[2,3-b]furan-3-ol	156928-09-5	DMF	-	-	NC	1	0.78	3	0.91	10	0.95							Glaxo SmithKline, Submitted by M.J. Olson
(3r,3as,6ar)-Hexahydrofuro-[2,3-b]furan-3-yl [(1s,2r)-3-[(1,3-benzodioxol-5-ylsulfonyl)(2-methylpropyl)-amino]-2-hydroxy-1-[[4-(2-methyl-4-thiazolyl)methoxy]phenyl]methyl]-propyl]carbamate	313682-08-5	DMF	-	-	NC	2.5	1.46	7.5	0.92	25	1.04							Glaxo SmithKline, Submitted by M.J. Olson
(3R6R)-3-(2,3-Dihydro-1h-inden-2-yl)-1-[(1r)-1-(2-methyl-1,3-oxazol-4-yl)-2-(4-morpholinyl)-2-oxoethyl]-6-[(1s)-1-methylpropyl]-2,5-piperazinedione	820957-38-8	DMF	-	-	NC	5	0.74	10	1.41	25	1.62							Glaxo SmithKline, Submitted by M.J. Olson

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(4r,5s)-(-)-1,5-Dimethyl-4-phenyl-2-imidazolidinone	92841-65-1	DMSO	-	-	NC	10	1.80	25	2.10	50	1.90							Glaxo SmithKline, Submitted by M.J. Olson
(4r,5s)-1,5-Dimethyl-3-(1-oxo-2-propenyl)-4-phenyl-2-imidazolidinone	139109-23-2	ACE	+	+	0.004	0.5	14.10	5	19.50	50	16.80							Glaxo SmithKline, Submitted by M.J. Olson
(4S)-1-(tert-Butoxycarbonyl)-4-fluoro-1-prolinamide	426844-22-6	DMF	-	-	NC	2.5	1.12	5	0.99	10	1.60							Glaxo SmithKline, Submitted by M.J. Olson
(4S)-1-(tert-Butoxycarbonyl)-4-fluoro-1-proline	203866-13-1	DMF	-	-	NC	5	0.88	10	0.82	25	1.29							Glaxo SmithKline, Submitted by M.J. Olson
(4S,5R)-1-[(1R,2R,3S)-3-(1,3-Benzodioxol-5-yl)-1-(2-benzyloxy-4-methoxyphenyl)-1-hydroxy-6-propoxy-2-indanoyl]-3,4-dimethyl-5-phenyl-2-imidazolidinone	190965-47-0	DMF	-	-	NC	0.5	0.78	5	1.14	10	1.39							Glaxo SmithKline, Submitted by M.J. Olson
(Alpha-r)-n-alpha-dimethyl-3,5-bis(trifluoro-methyl	334477-60-0	DMF	-	-	NC	10	1.32	25	1.41	50	1.63							Glaxo SmithKline, Submitted by M.J. Olson
(R,S)-3-Amino-2,3,4,5-tetrahydro-n-(1-methylethyl)-2,4-dioxo-n,5-diphenyl-1h-1,5-benzodiazepine-1-acetamide	184944-86-3	PG	-	-	NC	5	1.06	10	1.00	25	1.19							Glaxo SmithKline, Submitted by M.J. Olson
(s)-(-)-1-Phenylpropylamine	3789-59-1	AOO	-	-	NC	0.5	0.81	5	0.69	50	0.99							Glaxo SmithKline, Submitted by M.J. Olson
(S)-2-(4-Fluoro-2-methylphenyl)4-piperidinone (s)-alpha-hydroxybenzene-acetic acid salt	414910-13-7	DMF	-	-	NC	10	1.79	25	1.85	50	2.10							Glaxo SmithKline, Submitted by M.J. Olson

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[3aS-(3aAlpha, 4beta,5alpha, 6alpha,8beta, 9alpha,9abeta, 10S*)]-6-Ethenyldecahydro-5-hydroxy-4,6,9,10-tetramethyl-1-oxo-3a,9-propano-3aH-cyclopentacyclooct en-8-yl [(methylsulfonyl)-oxy]acetate	60924-38-1	DMF	-	-	NC	10	2.46	25	2.40	50	1.54							Glaxo SmithKline, Submitted by M.J. Olson
[4-(Ethoxymethyl)-2,6-dimethoxyphenyl]-boronic acid	591249-50-2	DMF	-	-	NC	10	0.87	25	0.58	50	1.00							Glaxo SmithKline, Submitted by M.J. Olson
[4S-[1(E),4A]alpha, 5alpha]]-1-[3-[2-[4-Methoxy-2-(phenylmethoxy)-benzoyl]-4-propoxyphenyl]-1-oxo-2-propenyl]-3,4-dimethyl-5-phenyl-2-imidazolidinone	190965-46-9	DMF	-	-	NC	0.05	0.88	0.5	0.59	5	0.56							Glaxo SmithKline, Submitted by M.J. Olson
1-(4-Ethoxyphenyl)-2-[4-(methylsulfonyl)phenyl]ethanone	346413-00-1	DMSO	-	-	NC	1	1.82	2.5	2.34	5	1.89							Glaxo SmithKline, Submitted by M.J. Olson
1,1-Dimethylethyl [(1s)-1-[bis(4-fluorophenyl)methyl]-2-[(2s,4s)-2-cyano-4-fluoro-1-pyrrolidinyl]-2-oxoethyl]carbamate	483368-24-7	AOO	-	-	NC	10	0.97	25	0.81	50	0.99							Glaxo SmithKline, Submitted by M.J. Olson
1,1-Dimethylethyl [(1s)-2-[4-[(2-methyl-4-thiazolyl)methoxy]phenyl]-1-(2s)-oxiranylethyl]carbamate	313680-92-1	DMF	-	-	NC	5	1.04	10	0.84	25	1.16							Glaxo SmithKline, Submitted by M.J. Olson

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1,1-Dimethylethyl 3-[[[(3s)-2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenyl amino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1h-1,5-benzodiazepin-3-yl]amino] carbonyl]amino] benzoate	305366-94-3	DMF	+	+	38	10	2.10	25	2.20	50	3.80							Glaxo SmithKline, Submitted by M.J. Olson
1,2,3,5,6,7-Hexahydro-2-thioxo-4h-cyclopentapyrimidin-4-one	35563-27-0	PG	-	-	NC	5	0.63	10	1.71	25	1.37							Glaxo SmithKline, Submitted by M.J. Olson
1,3-Benzodioxazole-5-sulphonyl chloride	115010-10-1	AOO	+	+	0.4	10	13.54	25	16.56	50	16.76							Glaxo SmithKline, Submitted by M.J. Olson
1-[3-(Cyclopentyl-oxy)-4-methoxyphenyl]-4-oxocyclohexane carbonitrile	152630-47-2	DMSO	-	-	NC	10	2.70	25	2.80	50	2.20							Glaxo SmithKline, Submitted by M.J. Olson
1-[5-[(4-Fluorophenyl)methyl]-2-furanyl]ethanone	280571-34-8	AOO	-	-	NC	0.5	1.00	5	1.00	50	1.20							Glaxo SmithKline, Submitted by M.J. Olson
14-Hydroxynormorphinone	84116-46-1	PG	+	+	8.4	5	1.20	10	3.88	25	6.24							Glaxo SmithKline, Submitted by M.J. Olson
2-(3,4-Dimethylphenyl)-5--methyl-2,4-dihydropyrazol-3-one	18048-64-1	DMF	+	+	IDR ³	2.5	4.41	7.5	4.82	25	8.46							Glaxo SmithKline, Submitted by M.J. Olson
2-(4-Ethoxyphenyl)-3-[4-(methylsulfonyl)phenyl]pyrazolo[1,5-b]pyridazine	221148-46-5	DMF	-	-	NC	5	0.98	10	0.97	25	0.94							Glaxo SmithKline, Submitted by M.J. Olson
2-(4-Oxopentyl)-1h-isindole-1,3(2h)-dione	3197-25-9	AOO	-	-	NC	0.25	0.58	2.5	1.54	25	0.67							Glaxo SmithKline, Submitted by M.J. Olson
2-(Benzyl)tert-butylamino)-1-(alpha,4-dihydroxym-tolyl)ethane	24085-03-8	DMF	-	-	NC	10	0.67	25	1.10	50	1.28							Glaxo SmithKline, Submitted by M.J. Olson

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2,3,4,5-Tetrahydro-n-(1-methylethyl)-2,4-dioxo-n,5-diphenyl-3-[(phenylmethoxy)imino]-1h-1,5-benzodiazepine-1-acetamide	305366-97-6	DMF	-	-	NC	5	1.18	10	1.76	25	1.67							Glaxo SmithKline, Submitted by M.J. Olson
2,3-Dimethyl-2h-indazol-6-amine	444731-72-0	DMF	-	-	NC	5	0.74	10	0.95	25	1.16							Glaxo SmithKline, Submitted by M.J. Olson
2,4-Dichloropyrimidine	3934-20-1	DMF	+	+	0.7	0.25	0.76	0.75	3.46	2.5	8.64							Glaxo SmithKline, Submitted by M.J. Olson
2,6-Dimethoxy-4-methyl-5-[3-(trifluoromethyl)phenoxy]-8-quinolinamine	106635-86-3	AOO	-	-	NC	0.5	2.30	5	2.10	50	1.80							Glaxo SmithKline, Submitted by M.J. Olson
2,6-Dimethoxy-4-methyl-8-nitro-5-[3-(trifluoromethyl)phenoxy]quinoline	189746-15-4	PG	+	+	3.5	3	2.90	10	4.29	30	5.34							Glaxo SmithKline, Submitted by M.J. Olson
2-[(Benzyloxy)imino]malonic acid	305366-96-5	AOO	-	-	NC	10	1.17	25	1.88	50	2.40							Glaxo SmithKline, Submitted by M.J. Olson
2-[1-(4-Bromophenyl)-1-phenylethoxy]-n,n-dimethylethanamine hydrochloride	13977-28-1	DMF	+	+	5.5	0.5	2.38	5	2.88	15	5.08							Glaxo SmithKline, Submitted by M.J. Olson
2-Amino-diphenylamine	534-85-0	AOO	+	+	0.5	10	10.20	25	12.40	50	7.70							Glaxo SmithKline, Submitted by M.J. Olson
2-Aminoethylmethylsulfone	49773-20-8	0.5% Tween 80 in H ₂ O	-	-	NC	10	0.40	25	0.30	50	0.30							Glaxo SmithKline, Submitted by M.J. Olson
2-Benzyl-tert-butylamino-3'-hydroxymethyl-4'-hydroxyacetophenone hydrochloride	24085-08-3	DMF	+	+	22	0.5	0.96	5	1.54	50	5.44							Glaxo SmithKline, Submitted by M.J. Olson
2-Bromo-5-hydroxy-benzaldehyde	2973-80-0	AOO	+	+	2.6	0.5	1.25	5	4.93	50	21.40							Glaxo SmithKline, Submitted by M.J. Olson

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2-Bromo-5-propoxybenzoic acid	190965-43-6	ACE	-	-	NC	0.5	0.60	5	0.70	50	1.10							Glaxo SmithKline, Submitted by M.J. Olson
2-Chloro-6-methoxy-4-methylquinoline	6340-55-2	DMF	-	-	NC	0.1	1.07	1	0.98	10	1.11							Glaxo SmithKline, Submitted by M.J. Olson
2-chloro-1-[(3-fluorophenyl)methoxy]-4-nitrobenzene	443882-99-3	AOO	+	+	IDR ³	5	3.96	10	2.62	25	3.22							Glaxo SmithKline, Submitted by M.J. Olson
2-Nitro-4-(propylthio)benzenamine	54393-89-4	AOO	Equiv	+	IDR ³	0.5	1.97 ⁴	5	1.34 ⁴	15	8.00 ⁵							Glaxo SmithKline, Submitted by M.J. Olson
3,4-Dichloroaniline hydrochloride	95-76-1	DMF	+	+	18	0.25	1.02	2.5	1.75	25	3.53							Glaxo SmithKline, Submitted by M.J. Olson
3-[(2r)-3-[[2-(2,3-Dihydro-1h-inden-2-yl)-1,1-dimethylethyl]amino]-2-hydroxypropoxy]-4,5-difluorobenzene propanoic acid	753449-67-1	DMF	-	-	NC	5	0.71	15	1.02	50	1.28							Glaxo SmithKline, Submitted by M.J. Olson
3'-[(2z)-[1-(3,4-Dimethylphenyl)-1,5-dihydro-3-methyl]-5-oxo-4h-pyrazol-4-ylidene]hydrazino]-2'-hydroxy-[1,1'-biphenyl]-3-carboxylic acid, compound with 2-aminoethanol (2:1)	496775-62-3	AOO	-	-	NC	5	1.38	15	1.05	50	0.84							Glaxo SmithKline, Submitted by M.J. Olson
3-[4-[(6-Bromohexyl)oxy]butyl]benzenesulfonamide	452342-04-0	AOO	-	-	NC	10	1.02	25	0.82	50	0.68							Glaxo SmithKline, Submitted by M.J. Olson
3-Chloro-4-fluorobenzoyl chloride	65055-17-6	PG	+	+	7.8	3	2.24	10	3.36	30	8.99							Glaxo SmithKline, Submitted by M.J. Olson
3-Fluoro-5-(3-pyridinyl)benzenamine	181633-36-3	DMSO	+	+	15	0.5	1.90	5	2.20	50	5.90							Glaxo SmithKline, Submitted by M.J. Olson
3-Hydroxy-2-phenyl-4-quinolinecarboxylic acid	485-89-2	DMSO	-	-	NC	0.05	0.56	0.5	0.79	5	1.04							Glaxo SmithKline, Submitted by M.J. Olson

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3-Hydroxy-4-methoxy-benzaldehyde	621-59-0	DMF	-	-	NC	0.25	0.75	2.5	1.15	25	1.35							Glaxo SmithKline, Submitted by M.J. Olson
3-Propoxybenzoic acid	190965-42-5	ACE	-	-	NC	0.5	1.10	5	1.20	50	1.10							Glaxo SmithKline, Submitted by M.J. Olson
4-(Bromomethyl)-benzoic acid ethyl ester	26496-94-6	AOO	+	+	IDR ³	0.5	11.73	5	12.87	50	ND ⁶							Glaxo SmithKline, Submitted by M.J. Olson
4'-(Trifluoromethyl)-[1,1'-biphenyl]-4-carboxaldehyde	90035-34-0	DMF	-	-	NC	1	1.36	3	1.55	10	2.58							Glaxo SmithKline, Submitted by M.J. Olson
4-[4-[[3(R)-1-Butyl-3-[(r)-cyclohexyl-hydroxymethyl]-2,5-dioxo-1,4,9-triazaspiro[5.5]undec-9-yl]methyl]phenoxy]benzoic acid	461443-59-4	DMSO	-	-	NC	2.5	1.07	5	1.27	10	1.63							Glaxo SmithKline, Submitted by M.J. Olson
4-Amino-3-nitrophenyl thiocyanate	54029-45-7	DMSO	+	+	0.8	0.5	2.30	1	3.32	5	3.55							Glaxo SmithKline, Submitted by M.J. Olson
4-Bromo-1-phthalimidopentane	59353-62-7	ACE	+	+	27	0.5	1.00	5	1.10	50	4.20							Glaxo SmithKline, Submitted by M.J. Olson
4-Chloro-6-iodoquinazoline	98556-31-1	AOO	+	+	IDR ³	5	11.30	10	9.30	25	17.30							Glaxo SmithKline, Submitted by M.J. Olson
4-Fluoro-2-pyrrolidine-carboxamide	748165-40-4	DMF	-	-	NC	10	1.22	25	1.15	50	1.03							Glaxo SmithKline, Submitted by M.J. Olson
4-Iodo-1-phthalimido-pentane	63460-47-9	ACE	+	+	5.0	0.5	1.70	5	3.00	50	9.50							Glaxo SmithKline, Submitted by M.J. Olson
5-[[4-[(2,3-Dimethyl-2h-indazol-6-yl)-methylamino]-2-pyrimidinyl]amino]-2-methylbenzene-sulfonamide	444731-52-6	AOO	-	-	NC	5	1.13	10	0.91	25	0.91							Glaxo SmithKline, Submitted by M.J. Olson
5-Amino-2-methylbenzene-sulfonamide	6973-09-7	DMF	-	-	NC	5	1.36	10	1.12	25	1.42							Glaxo SmithKline, Submitted by M.J. Olson

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5-Chloro-2,6-dimethoxy-4-methyl-8-nitroquinoline	189746-21-2	DMSO	+	+	IDR ³	0.5	8.00	5	7.00	10	7.50							Glaxo SmithKline, Submitted by M.J. Olson
5-Chloro-2,6-dimethoxy-4-methylquinoline	189746-19-8	DMSO	-	-	NC	0.5	0.90	5	0.70	25	1.00							Glaxo SmithKline, Submitted by M.J. Olson
5'-Chloro-2'-hydroxy-3'-nitro-[1,1'-biphenyl]-3-carboxylic acid	376592-58-4	DMF	+	+	20	5	1.37	15	2.83	50	3.96							Glaxo SmithKline, Submitted by M.J. Olson
5-Chloro-6-methoxy-4-methyl-8-nitro-2(1h)quinolinone	189746-23-4	PG	+	+	IDR ³	2.5	10.82	5	9.86	10	10.72							Glaxo SmithKline, Submitted by M.J. Olson
5-Methoxy-2-nitro-4-(trifluoromethyl) benzene acetonitrile	178896-77-0	DMSO	-	-	NC	0.5	1.30	5	1.50	50	1.60							Glaxo SmithKline, Submitted by M.J. Olson
5-Methoxy-6-(trifluoromethyl)-2,3-dihydro-1h-indole	178896-79-2	DMSO	+	+	37	0.5	1.10	5	1.30	50	3.70							Glaxo SmithKline, Submitted by M.J. Olson
6-(Diethylamino)-1-hexanol	06947-12-2	PG	+	+	10	3	0.79	10	2.92	30	25.50							Glaxo SmithKline, Submitted by M.J. Olson
6-(Trifluoromethyl)-2,3-dihydro-5-methyl-1h-indole, hydrochloride	280121-24-6	ETOH (100%)	-	-	NC	0.5	1.10	5	1.00	50	1.20							Glaxo SmithKline, Submitted by M.J. Olson
6-[(2-Methyl-3-pyridinyl)oxy]-3-pyridinamine	181633-42-1	DMSO	+	+	45	0.5	1.00	5	1.40	50	3.20							Glaxo SmithKline, Submitted by M.J. Olson
6-Chloro-1-hexanol	2009-83-8	AOO	-	-	NC	5	2.35	15	1.66	50	1.92							Glaxo SmithKline, Submitted by M.J. Olson
6-Diethylaminoethyl bromide hydrobromide	64993-14-2	PG	+	+	5.3	3	1.76	10	5.46	30	14.69							Glaxo SmithKline, Submitted by M.J. Olson
6-Iodo-quinazolin-4-ol	16064-08-7	DMF	-	-	NC	1	0.72	2.5	1.16	5	0.93							Glaxo SmithKline, Submitted by M.J. Olson
6-Methoxy-4-methyl-2(1H)-quinolinone	5342-23-4	PG	-	-	NC	3	1.21	10	1.49	30	1.32							Glaxo SmithKline, Submitted by M.J. Olson

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7-[(4z)-3-(Aminomethyl)-4-(methoxyimino)-1-pyrrolidinyl]-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylic acid, monomethanesulfonate	210353-53-0	DMSO	+	+	8.6	0.1	0.75	1	1.38	10	3.30							Glaxo SmithKline, Submitted by M.J. Olson
8-[(4-Phthalimido-1-methylbutyl)amino]-2,6-dimethoxy-4-methyl-5-(3-trifluoromethylphenoxy)quinoline	106635-87-4	PG	-	-	NC	3	2.22	10	1.50	30	1.49							Glaxo SmithKline, Submitted by M.J. Olson
8-Amino-6-methoxy-4-methylquinoline	57514-21-3	PG	-	-	NC	3	1.23	10	2.83	30	2.50							Glaxo SmithKline, Submitted by M.J. Olson
8-Chloro-3-pentyl-3,7-dihydro-1h-purine-2,6-dione	862892-90-8	DMF	+	+	32	5	2.00	15	0.85	50	5.29							Glaxo SmithKline, Submitted by M.J. Olson
8-Hydroxy-5-[(1r)-1-hydroxy-2-[[2-[4-[(6-methoxy[1,1'-biphenyl]-3-yl)amino]phenyl]-ethyl]amino]ethyl]-2(1h)-quinolinone	530084-87-8	DMF	-	-	NC	5	0.96	10	2.34	25	1.58							Glaxo SmithKline, Submitted by M.J. Olson
Adipic acid	124-04-9	DMSO	-	-	NC	10	1.01	25	0.93	50	0.79							Glaxo SmithKline, Submitted by M.J. Olson
Alpha-(p-toluenesulfonyl)-4-fluorobenzylisocyanide	165806-95-1	DMF	+	+	45	0.5	4.72	5	2.78	50	3.03							Glaxo SmithKline, Submitted by M.J. Olson
Anthranilic acid	118-92-3	AOO	-	-	NC	10	0.90	25	1.10	50	1.40							Glaxo SmithKline, Submitted by M.J. Olson
cis-4-Cyano-4-[3-(cyclopentyloxy)-4-methoxyphenyl]cyclohexanecarboxylic acid	153259-65-5	DMSO	-	-	NC	0.5	1.16	5	1.27	10	1.28							Glaxo SmithKline, Submitted by M.J. Olson
Cytosine hemihydrate	71-30-7	PG	-	-	NC	5	0.40	10	0.90	25	0.70							Glaxo SmithKline, Submitted by M.J. Olson

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Dimethyl 4-cyano-4-(3-cyclopentyloxy-4-methoxyphenyl)-pimelate	152630-48-3	AOO	-	-	NC	0.5	1.66	5	1.59	50	1.76							Glaxo SmithKline, Submitted by M.J. Olson
Dimethyl carbonate	616-38-6	AOO	-	-	NC	0.5	0.64	5	0.69	50	1.71							Glaxo SmithKline, Submitted by M.J. Olson
Endo-tropine-3-mesylate	35130-97-3	DMF	+	+	4.4	5	3.45	10	5.98	25	25.06							Glaxo SmithKline, Submitted by M.J. Olson
Ethyl (3-endo)-8-methyl-8-azabicyclo[3.2.1]octane-3-acetate	56880-11-6	DMF	+	+	5.5	10	6.77	25	12.58	50	ND ^b							Glaxo SmithKline, Submitted by M.J. Olson
Ethyl (z)-alpha-[[2-(1,1-dimethylethoxy)-1,1-dimethyl-2-oxoethoxy]imino]-2-[(triphenylmethyl)amino]-4-thiazoleacetate	68672-65-1	Butanone	-	-	NC	2.5	0.80	5	1.32	10	0.92							Glaxo SmithKline, Submitted by M.J. Olson
Ethyl 1h-1,2,4-triazole-3-carboxylate	64922-04-9	DMF	-	-	NC	0.25	1.00	2.5	1.20	25	1.00							Glaxo SmithKline, Submitted by M.J. Olson
Ethyl 2,6-dichloro-5-fluoro-beta-oxo-3-pyridinepropanoate	96568-04-6	AOO	-	-	NC	0.25	0.59	2.5	1.33	25	1.97							Glaxo SmithKline, Submitted by M.J. Olson
Ethyl 4-iodobenzoate	51934-41-9	AOO	+	+	8.0	0.5	1.10	5	2.20	50	14.30							Glaxo SmithKline, Submitted by M.J. Olson
Isopropyl dicyandiamide	35695-36-4	DMF	-	-	NC	0.25	1.36	2.5	1.35	25	1.24							Glaxo SmithKline, Submitted by M.J. Olson
m-Chloropropiophenone	34841-35-5	AOO	-	-	NC	10	0.86	25	0.73	50	1.25							Glaxo SmithKline, Submitted by M.J. Olson
Methyl 4-(bromomethyl)benzoate	2417-72-3	AOO	+	+	IDR ³	0.5	26.83	5	18.47	50	ND ^b							Glaxo SmithKline, Submitted by M.J. Olson
n-(2-Chloro-4-pyrimidinyl)-2,3-dimethyl-2h-indazol-6-amine	444731-74-2	DMF	-	-	NC	1	0.80	2.5	0.74	5	1.07							Glaxo SmithKline, Submitted by M.J. Olson

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n-(2-Chloro-4-pyrimidinyl)-n,2,3-trimethyl-2h-indazol-6-amine	444731-75-3	DMF	-	-	NC	1	1.28	2.5	1.47	5	2.15							Glaxo SmithKline, Submitted by M.J. Olson
n-(3,4-Dichlorophenyl)-n'-(1-methylethyl)-imidodicarbonimidic diamide monohydrochloride	15537-76-5	DMF	+	+	1.3	0.25	1.64	2.5	4.61	25	ND ^b							Glaxo SmithKline, Submitted by M.J. Olson
n-(4-Methoxyphenyl)-3-oxobutanamide	5437-98-9	PG	+	+	2.2	3	3.10	10	3.49	30	10.33							Glaxo SmithKline, Submitted by M.J. Olson
n-[(1,1-Dimethylethoxy)-carbonyl]-l-tyrosine, ethyl ester	72594-77-5	AOO	-	-	NC	10	1.18	25	1.09	50	0.64							Glaxo SmithKline, Submitted by M.J. Olson
n-[(1-Butyl-4-piperidinyl)methyl]-3,4-dihydro-2h-[1,3]oxazino[3,2-a]indole-10-carboxamide	152811-62-6	AOO	-	-	NC	0.5	0.80	5	1.20	25	1.30							Glaxo SmithKline, Submitted by M.J. Olson
n-[2-(Diethylamino)ethyl]-2-[[[4-fluorophenyl)methyl]thio]-4,5,6,7-tetrahydro-4-oxo-n-[[4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl]methyl]-1h-cyclopentapyrimidine-1-acetamide	356057-34-6	EtOH/dH ₂ O (4:1)	+	+	11	5	1.11	10	2.43	25	12.71							Glaxo SmithKline, Submitted by M.J. Olson
n-[2-Benzyloxy-5-(2-bromo-1-hydroxy-ethyl)-phenyl]-formamide	201677-59-0	DMF	-	-	NC	10	0.98	25	0.68	50	0.97							Glaxo SmithKline, Submitted by M.J. Olson
n-[(1,1-Dimethylethyl)oxy]carbonyl]-4-fluoro-beta-(4-fluorophenyl)-l-phenylalanine	481055-29-2	DMF	-	-	NC	10	1.47	25	2.41	50	2.28							Glaxo SmithKline, Submitted by M.J. Olson
1-Aminopyridazinium iodide	35073-04-2	DMF	-	-	NC	10	1.17	25	1.43	50	1.25							Glaxo SmithKline, Submitted by M.J. Olson

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n-Isopropyl-n-phenyl-2-(2-phenylamino-phenylamino)-acetamide	161455-90-9	DMF	+	+	2.1	2.5	3.80	5	7.30	10	6.60							Glaxo SmithKline, Submitted by M.J. Olson
Oripavine	467-04-9	DMF	+	+	8.6	2.5	1.90	5	2.50	10	3.20							Glaxo SmithKline, Submitted by M.J. Olson
Phenylmethyl 2-(4-fluoro-2-methylphenyl)-4-oxo-3,4-dihydro-1(2h)-pyridine-carboxylate	414909-98-1	DMF	-	-	NC	10	1.67	25	1.85	50	1.47							Glaxo SmithKline, Submitted by M.J. Olson
rel-(3r,3as,6ar)-Hexahydrofuro[2,3-b]furan-3-yl 4-nitrophenyl carbonate	252873-35-1	DMF	+	+	IDR ³	2.5	3.48	7.5	3.40	25	3.54							Glaxo SmithKline, Submitted by M.J. Olson
Sodium ethyl xanthate	140-90-9	PG	+	+	7.3	5	1.57	10	4.70	25	9.42							Glaxo SmithKline, Submitted by M.J. Olson
tert-Butyl-3-aminobenzoate	92146-82-2	DMF	-	-	NC	10	1.24	25	1.02	50	1.08							Glaxo SmithKline, Submitted by M.J. Olson
Trienol	13504-15-9	DMF	-	-	NC	5	1.40	10	1.10	25	1.00							Glaxo SmithKline, Submitted by M.J. Olson
Veratraldehyde	120-14-9	AOO	+	+	3.2	0.5	2.63	5	3.24	50	3.47							Glaxo SmithKline, Submitted by M.J. Olson
Basil oil	8015-73-4	EtOH/DEP (1:3)	+	+	IDR ³	2.5	3.00	5.0	3.00	10.0	8.00	25.0	17.60	50.0	25.20			Lalko & Api (2006), Submitted by A. Api (RIFM)
Citral	5392-40-5	EtOH/DEP (1:3)	+	+	6.3	2.5	2.80	5.0	2.30	10.0	5.10	25.0	11.40	50.0	22.10			Lalko & Api (2006), Submitted by A. Api (RIFM)
Citronella oil	8000-29-1	EtOH/DEP (1:3)	-	-	NC	2.5	1.40	5.0	0.90	10.0	1.20	25.0	1.20	50.0	2.70			Lalko & Api (2006), Submitted by A. Api (RIFM)
Clove bud oil	8000-34-8	EtOH/DEP (1:3)	+	+	7.1	1.0	1.10	2.5	1.80	5.0	2.50	10.0	3.70	25.0	5.90			Lalko & Api (2006), Submitted by A. Api (RIFM)
Clove leaf oil	8015-97-2	EtOH/DEP (1:3)	+	+	8.0	2.5	1.60	5.0	1.50	10.0	4.00	25.0	9.50	50.0	11.40			Lalko & Api (2006), Submitted by A. Api (RIFM)

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Clove stem oil	8015-98-3	EtOH/DEP (1:3)	+	+	7.0	1.0	1.60	2.5	1.70	5.0	2.20	10.0	4.20	25.0	8.90			Lalko & Api (2006), Submitted by A. Api (RIFM)
Eugenol	97-53-0	EtOH/DEP (1:3)	+	+	5.5	2.5	1.20	5.0	2.70	10.0	6.00	25.0	14.30	50.0	19.40			Lalko & Api (2006), Submitted by A. Api (RIFM)
Geraniol	106-24-1	EtOH/DEP (1:3)	+	+	12	2.5	1.70	5.0	2.40	10.0	2.80	25.0	4.80	50.0	6.00			Lalko & Api (2006), Submitted by A. Api (RIFM)
Geranium oil	8000-46-2	EtOH/DEP (1:3)	-	-	NC	2.5	1.20	5.0	0.70	10.0	1.70	25.0	1.80	50.0	2.80			Lalko & Api (2006), Submitted by A. Api (RIFM)
Jasmine absolute (Grandiflorum)	8022-96-6	EtOH/DEP (1:3)	+	+	5.9	1.0	1.20	2.5	1.80	5.0	2.00	10.0	7.40	25.0	11.80			Lalko & Api (2006), Submitted by A. Api (RIFM)
Jasmine absolute (Sambac)	8022-96-6	EtOH/DEP (1:3)	+	+	36	10	1.70	25.0	2.50	50.0	3.60	75.0	10.80	100.0	16.20			Lalko & Api (2006), Submitted by A. Api (RIFM)
Lemongrass oil	8007-02-1	EtOH/DEP (1:3)	+	+	6.5	2.5	0.90	5.0	2.10	10.0	5.10	25.0	10.30	50.0	13.10			Lalko & Api (2006), Submitted by A. Api (RIFM)
Litsea cubeba oil	68855-99-2	EtOH/DEP (1:3)	+	+	8.5	2.5	2.00	5.0	2.30	10.0	3.30	25.0	7.90	50.0	16.00			Lalko & Api (2006), Submitted by A. Api (RIFM)
Palmarosa oil	8014-19-5	EtOH/DEP (1:3)	+	+	9.5	2.5	1.10	5.0	2.10	10.0	3.10	25.0	3.60	50.0	5.00			Lalko & Api (2006), Submitted by A. Api (RIFM)
Spearmint oil	68917-46-4	EtOH/DEP (1:3)	+	+	8.2	0.5	1.20	1.0	1.10	2.5	1.20	5.0	1.90	10.0	3.60			Lalko & Api (2006), Submitted by A. Api (RIFM)
Ylang Ylang (Extra)	8006-81-3	EtOH/DEP (1:3)	+	+	6.8	0.5	1.50	1.0	1.40	2.5	2.10	5.0	2.50	10.0	3.90			Lalko & Api (2006), Submitted by A. Api (RIFM)
Ylang Ylang (III)	8006-81-3	EtOH/DEP (1:3)	-	-	NC	0.5	1.30	1.0	1.70	2.5	2.10	5.0	2.60	10.0	2.60			Lalko & Api (2006), Submitted by A. Api (RIFM)
(1R,4R)-4-Isopropenyl-1-methyl-2-methylene-cyclohexane		AOO	-	-	NC	1	1.30	5	1.80	10	1.20	15	2.30	25	2.90			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick

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(3S,6R)-3-isopropyl-6-methylcyclohexene	5113-93-9	AOO	-	-	NC	1	0.84	10	1.00	25	2.90							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
(4Z)-2-Methyl-6-methyloct-4-ene			-	-	NC	1	1.10	5	0.87	10	0.78	15	0.89	25	2.10			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
(5R)-5-Isopropenyl-2-methyl-1-methylene-2-cyclohexene		AOO	+	+	7.3	0.5	0.94	5	1.90	15	6.60							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
2,2-bis-[4-(2-hydroxy-3-methacryloxypropoxy)phenyl]propane	1565-94-2	AOO	+	+	45	35	2.00	75	5.90									LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
2,4-Diaminophenoxyethanol HCl	66422-95-5	AOO	+	+	5.5	1	1.60	2.5	1.60	5	2.70	10	5.70	25	8.30			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
2,4-Hexadienal	142-83-6	AOO	+	+	3.5	0.5	0.90	1	1.50	2.5	2.20	5	4.20	10	14.80			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
3,4-epoxycyclohexylethyl-cyclopoly-methylsiloxane		AOO	-	-	NC	50	1.20	100	1.20									LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
4,4-Dibromobenzil	35578-47-3	AOO	+	+	21	5	1.50	10	1.60	25	3.60	50	5.70					LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick

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4-Isopropyl-1-methylene-cyclohexane		AOO	-	-	NC	1	1.20	10	0.71	25	1.40							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
5-Methyl-2-phenyl-2-hexenal	21834-92-4	AOO	+	+	4.4	0.5	1.00	1.0	1.30	2.5	0.50	5	3.80	10	17.70			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
a-Phellandrene	99-83-2	AOO	+	+	5.4	1.0	1.10	10	5.00	25	28.00							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
a-Terpinene	99-86-5	AOO	+	+	8.9	1	1.1	5	1.5	10	3.40	15	8.90	25	23.00			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Bandrowski's base	20048-27-5	AOO	+	+	0.02	0.01	1.10	0.025	3.10	0.05	5.70	0.1	6.50	0.25	5.60			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
beta-Phenyl-cinnamaldehyde	1210-39-5	AOO	+	+	0.6	0.1	2.00	0.25	2.30	0.5	1.90	1	5.90	2.5	10.60			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Bis-3,4-epoxycyclohexyl-ethyl-phenyl-methylsilane (Ph-Sil)		AOO	+	+	16	25	3.70	35	4.20	50	7.90							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
b-Phellandrene	555-10-2	AOO	+	+	NC	1.0	1.10	10	4.80	20	23.00							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick

Substance Name	CASRN	Vehicle	rLLNA ¹	Trad. LLNA ¹	EC3 ²	1 Conc. (%)	1 SI	2 Conc. (%)	2 SI	3 Conc. (%)	3 SI	4 Conc. (%)	4 SI	5 Conc. (%)	5 SI	6 Conc. (%)	6 SI	Data Source
b-Terpinene	99-84-3	AOO	-	-	NC	1	1.4	10	1.30	25	2.1							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Butyl acrylate	141-32-2	AOO	+	+	11	1	0.70	2.5	1.30	5	1.50	10	2.50	25	8.70			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Chlorothalonil	1897-45-6	DMF	+	+	0.004	0.003	2.10	0.01	9.40	0.03	13.80	0.1	18.40	0.3	27.20			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Ethyl hexyl acrylate	103-11-7	AOO	+	+	9.7	0.5	1.10	1	1.20	2.5	0.90	5	1.20	10	3.10			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Iodopropynyl butylcarbamate	87977-28-4	AOO	+	+	0.9	0.1	0.70	1	3.40	5	4.20	10	12.00					LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Linalool alcohol	78-70-6	AOO	-	-	NC	1	1.00	10	1.30	30	1.30							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Linalool aldehyde		AOO	+	+	9.5	1	1.20	5	2.00	15	4.20							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Methyl acrylate	96-33-3	AOO	+	+	20	1	0.80	2.5	0.80	5	1.30	10	1.60	25	3.80			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick

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Substance Name	CASRN	Vehicle	rLLNA ¹	Trad. LLNA ¹	EC3 ²	1 Conc. (%)	1 SI	2 Conc. (%)	2 SI	3 Conc. (%)	3 SI	4 Conc. (%)	4 SI	5 Conc. (%)	5 SI	6 Conc. (%)	6 SI	Data Source
Methyl pyruvate	600-22-6	AOO	+	+	2.4	1.0	1.20	2.5	3.10	5.0	4.70	10	8.00					LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Methyl methacrylate	80-62-6	AOO	+	+	90	10	1.40	30	1.50	50	1.50	75	2.10	100	3.60			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Norbomene fluoroalcohol	305815-63-8	AOO	+	+	46	5.0	0.70	10	0.80	25.0	1.90	50	3.20	100	3.70			LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
R-Carvone	2244-16-8	AOO	+	+	13	6	1.30	12	2.60	20	6.20							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
R-Carvoxime	2051-55-0	AOO	+	+	0.6	0.1	2.10	1	3.70	5	8.10							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
Trans-2-methyl-2-butenal	497-03-0	AOO	-	-	NC	10	1.50	25	1.00	50	1.80							LLNA/EC3 Validation Study, Submitted by D. Basketter, I. Kimber, and F. Gerberick
1-Chloro-2-dinitrobenzene	97-00-7	AOO	+	+	0.1	0.01	1.17	0.025	1.12	0.05	1.93	0.10	1.95	0.25	7.10			NTP Study, Submitted by D. Germolec
5-Amino-O-Cresol	2835-95-2	AOO	+	+	7.7	2.5	1.45	5.00	2.77	10.00	3.19							NTP Study, Submitted by D. Germolec
Atrazine	1912-24-9	ACE	-	-	NC	10	1.29	20.00	1.38	30.00	0.76							NTP Study, Submitted by D. Germolec
Azithromycin	83905-01-5	ACE	-	+	IDR ³	10	3.72	20.00	1.54	40.00	2.10							NTP Study, Submitted by D. Germolec

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Butyl acrylate	141-32-2	ACE	+	+	24	10	1.00	20.00	2.18	30.00	4.07							NTP Study, Submitted by D. Germolec
Clarithromycin	81103-11-9	ACE	-	-	NC	1	1.78	2.00	1.03	4.00	1.18							NTP Study, Submitted by D. Germolec
Dicyclohexylcarbodiimide	538-75-0	ACE	+	+	0.057	0.006	1.03	0.03	1.71	0.06	3.16							NTP Study, Submitted by D. Germolec
Ethyl acrylate	140-88-5	ACE	-	-	NC	10	0.89	20.00	1.19	30.00	0.91							NTP Study, Submitted by D. Germolec
Ethyl-2-(Hydroxymethyl)-1,3-Propanediol Triacrylate		ACE	+	+	0.13	0.3	1.00	0.10	1.52	0.15	4.13	0.30	4.59					NTP Study, Submitted by D. Germolec
Methyl salicylate	119-36-8	AOO	-	-	NC	1	0.86	2.50	1.19	5.00	1.16	10.00	1.41	20.00	1.72			NTP Study, Submitted by D. Germolec
Pentaerythritol Triacrylate	3524-68-3	ACE	-	-	NC	0.005	1.19	0.01	0.92	0.05	1.68	0.10	2.43					NTP Study, Submitted by D. Germolec
Potassium dichromate	7778-50-9	DMSO	+	+	0.2	0.025	1.21	0.05	1.84	0.10	2.22	0.25	3.39					NTP Study, Submitted by D. Germolec
Rifamycin SV	14897-39-3	AOO	-	-	NC	3	0.94	10.00	1.02	30.00	1.33							NTP Study, Submitted by D. Germolec
Sodium metasilicate	6834-92-0	EtOH (15%)	-	-	NC	2	0.87	4.00	1.40	6.00	1.29							NTP Study, Submitted by D. Germolec
Trimethylolpropane Triacrylate	15625-89-5	ACE	-	-	NC	0.05	0.96	0.10	0.87	0.25	1.62							NTP Study, Submitted by D. Germolec
2,4-Dinitrobenzene sulfonic acid	89-02-1	H ₂ O	+	+	15	1	1.70	10	1.50	20	4.40							Ryan et al. (2002)
2,4-Dinitrobenzene sulfonic acid	89-02-1	Pluronic L92	+	+	6.4	1	0.90	10	4.40	20	11.60							Ryan et al. (2002)
2,4-Dinitrobenzene sulfonic acid	89-02-1	DMF	+	+	0.8	1	4.00	10	16.30	20	18.50							Ryan et al. (2002)
2,4-Dinitrobenzene sulfonic acid	89-02-1	DMSO	+	+	2.0	1	1.70	10	13.70	20	16.10							Ryan et al. (2002)
Formaldehyde	50-00-0	H ₂ O	+	+	15	1	1.20	10	2.50	20	3.60							Ryan et al. (2002)
Formaldehyde	50-00-0	Pluronic L92	+	+	4.2	1	2.00	10	4.80	20	8.80							Ryan et al. (2002)
Formaldehyde	50-00-0	DMF	+	+	0.3	1	6.70	10	13.20	20	17.70							Ryan et al. (2002)
Formaldehyde	50-00-0	DMSO	+	+	0.3	1	7.50	10	16.00	20	17.60							Ryan et al. (2002)

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Nickel sulfate	7786-81-4	Pluronic L92 (1%)	-	+	2.5	0.25	2.00	0.5	2.40	1	2.80	2.5	3.00	5	2.30			Ryan et al. (2002)
Nickel sulfate	7786-81-4	DMF	-	-	NC	0.25	0.90	0.5	1.10	1	1.60	2.5	1.60	5	2.20			Ryan et al. (2002)
Nickel sulfate	7786-81-4	DMSO	+	+	4.8	0.25	1.30	0.5	1.40	1	1.40	2.5	1.80	5	3.10			Ryan et al. (2002)
Pluronic L92\		H ₂ O	-	-	NC	1	1.30	2.5	1.00	5	1.00	10	0.80	25	0.80	50	2	Ryan et al. (2002)
Potassium dichromate	7778-50-9	Pluronic L92 (1%)	+	+	0.2	0.025	1.10	0.05	1.10	0.1	1.40	0.25	4.90	0.5	5.40			Ryan et al. (2002)
Potassium dichromate	7778-50-9	DMF	+	+	0.03	0.025	2.90	0.05	4.30	0.1	9.10	0.25	15.10	0.5	22.60			Ryan et al. (2002)
Potassium dichromate	7778-50-9	DMSO	+	+	0.05	0.025	1.40	0.05	2.50	0.1	9.50	0.25	25.90	0.5	10.10			Ryan et al. (2002)

Abbreviations: ACE = acetone; AOO = acetone: olive oil (4:1 by volume); BGIA = Berufsgenossenschaftliches Institut für Arbeitsschutz (German Institute for Occupational Safety and Health); CASRN = Chemical Abstract Service Registry Number; CESIO = Comité Européen des Agents de Surface et de Leurs Intermédiaires Organiques (European Committee of Surfactants and their Organic Intermediates; Conc. = concentration; DBP = dibutyl phosphate; DEP = diethyl phthalate; dH₂O = distilled water; DMF = dimethylformamide; DMSO = dimethyl sulfoxide; ECPA = European Crop Protection Association; EFfCI = European Federation for Cosmetic Ingredients; ECPA = European Crop Protection Association; EtOH = ethanol; H₂O = water; LLNA = Local Lymph Node Assay; MEK = methyl ethyl ketone; NC = not calculated because no SI value was ≥ 3 (i.e., substance was a nonsensitizer); ND = no data; NTP = National Toxicology Program; PA/ H₂O = pluronic acid/ H₂O (1%); PG = propylene glycol; rLLNA = Reduced Local Lymph Node Assay; RIFM = Research Institute for Fragrance Materials; SI = stimulation index; Trad. = traditional

¹ "+" = Sensitizer; "-" = Non-sensitizer

² EC3 represents the estimated concentration needed to produce a stimulation index of three (i.e., a three fold increase in lymphocyte proliferation is observed for the test substance versus the vehicle control substance) and was calculated using the methods described in Ryan et al. (2007).

³ IDR indicates an insufficient dose response to calculate an EC3 value using the methods in Ryan et al. (2007)

⁴ Result of initial study

⁵ Result of second study

⁶ Data not obtained due to toxicity