

LabCyte EPI-MODEL24を用いた皮膚刺激性試験プロトコール法

試験結果 (54 化学物質)

NI: non-irritant 非刺激性

I: irritant 刺激性

No.	化合物		In vivo score	In vivo class (GHS分類)	EPI-MODEL24を用いた皮膚刺激性試験結果			
	名称	CAS number			生細胞率 (%) (対陰性対照)		In vitro Class I/NI	
					Run	Mean ± SD		
1	1-bromo-4-chlorobutane	6940-78-9	0	NI	1	17.3 ± 4.4	I	I
					2	23.7 ± 1.5	I	
					3	18.6 ± 2.1	I	
2	diethyl phthalate	84-66-2	0	NI	1	104.3 ± 4.4	NI	NI
					2	103.1 ± 1.5	NI	
					3	55.4 ± 13.8	NI	
3	di-propylene glycol	25265-71-8	0	NI	1	109.9 ± 2.0	NI	NI
					2	100.2 ± 10.2	NI	
					3	92.9 ± 12.2	NI	
4	naphthalen acetic acid	86-87-3	0	NI	1	92.7 ± 1.2	NI	NI
					2	107.8 ± 2.0	NI	
					3	98.5 ± 3.8	NI	
5	3-ChloronitroBenzene	121-73-3	0	NI	1	104.3 ± 4.4	NI	NI
					2	98.0 ± 2.2	NI	
					3	95.2 ± 6.9	NI	
6	3,3-Dithiodipropionic Acid	1119-62-6	0	NI	1	100.0 ± 5.6	NI	NI
					2	98.9 ± 2.5	NI	
					3	89.9 ± 10.1	NI	
7	4,4-Methylenebis (2,6-di-tert-butylphenol)	118-82-1	0	NI	1	103.9 ± 10.6	NI	NI
					2	100.0 ± 3.5	NI	
					3	100.0 ± 9.9	NI	
8	4-Amino-1,2,4-Triazole	584-13-4	0	NI	1	101.0 ± 6.9	NI	NI
					2	97.4 ± 6.7	NI	
					3	98.8 ± 8.4	NI	
9	Benzyl Benzoate	120-51-4	0	NI	1	105.7 ± 2.0	NI	NI
					2	99.6 ± 3.2	NI	
					3	100.3 ± 10.1	NI	
10	Sodium Bicarbonate	144-55-8	0	NI	1	99.6 ± 3.7	NI	NI
					2	100.0 ± 5.5	NI	
					3	100.3 ± 12.4	NI	
11	Erucamide	112-84-5	0	NI	1	102.5 ± 2.2	NI	NI
					2	92.7 ± 2.8	NI	
					3	90.0 ± 11.0	NI	
12	1,5-hexadiene	592-42-7	0	NI	1	85.6 ± 12.2	NI	NI
					2	92.5 ± 7.2	NI	
					3	95.6 ± 3.8	NI	
13	Polyethylene glycol 400	25322-68-3	0	NI	1	106.6 ± 8.7	NI	NI
					2	98.2 ± 5.4	NI	
					3	103.2 ± 4.3	NI	
14	Glycerol	56-81-5	0	NI	1	125.7 ± 9.0	NI	NI
					2	98.1 ± 6.5	NI	
					3	103.3 ± 6.5	NI	
15	3,3-Dimethylpentane	562-49-2	0	NI	1	72.3 ± 3.2	NI	NI
					2	76.3 ± 9.7	NI	
					3	90.8 ± 1.9	NI	
16	allyl phenoxy-acetate	7493-74-5	0.3	NI	1	94.7 ± 1.8	NI	NI
					2	96.3 ± 3.6	NI	
					3	56.0 ± 3.8	NI	
17	Isopropanol	67-63-0	0.3	NI	1	83.5 ± 5.6	NI	NI
					2	87.7 ± 2.8	NI	
					3	82.7 ± 8.5	NI	
18	Benzyl Salicylate	118-58-1	0.3	NI	1	93.6 ± 16.4	NI	NI
					2	98.2 ± 3.6	NI	
					3	99.9 ± 9.7	NI	
19	Lauric Acid	143-07-7	0.3	NI	1	94.0 ± 4.0	NI	NI
					2	109.2 ± 7.4	NI	
					3	110.0 ± 6.3	NI	
20	4-methyl-thio-benzaldehyde	3446-89-7	1	NI	1	24.6 ± 5.8	I	I
					2	21.4 ± 1.1	I	
					3	21.8 ± 0.8	I	
21	Methyl Stearate	112-61-8	1	NI	1	98.6 ± 4.8	NI	NI
					2	113.1 ± 4.5	NI	
					3	101.5 ± 4.9	NI	
22	Benzyl Acetate	140-11-4	1	NI	1	11.3 ± 2.7	I	I
					2	29.8 ± 4.7	I	
					3	37.4 ± 8.0	I	
23	Hydroxycitronellal	107-75-5	1	NI	1	19.8 ± 11.2	I	I
					2	20.4 ± 1.8	I	
					3	32.3 ± 6.0	I	
24	Isopropyl Myristate	110-27-0	1	NI	1	107.9 ± 3.7	NI	NI
					2	97.3 ± 5.2	NI	
					3	97.2 ± 12.4	NI	
25	Isopropyl Palmitate	142-91-6	1	NI	1	104.1 ± 10.6	NI	NI
					2	102.5 ± 1.3	NI	
					3	115.9 ± 2.2	NI	
26	n-Butyl Propionate	590-01-2	1	NI	1	23.1 ± 4.7	I	I
					2	41.2 ± 6.4	I	
					3	45.9 ± 6.4	I	
27	Sodium Bisulphite	7631-90-5	1	NI	1	11.1 ± 5.5	I	NI
					2	61.2 ± 6.8	NI	
					3	74.7 ± 9.7	NI	
28	Benzyl Alcohol	100-51-6	1.3	NI	1	5.6 ± 1.3	I	I
					2	17.5 ± 4.9	I	
					3	17.8 ± 2.0	I	
29	allyl heptanoate	142-19-8	1.7	NI	1	95.6 ± 5.7	NI	NI
					2	108.9 ± 10.7	NI	
					3	104.6 ± 3.3	NI	
30	heptyl butyrate	5870-93-9	1.7	NI	1	105.9 ± 2.0	NI	NI
					2	108.8 ± 10.4	NI	
					3	109.7 ± 1.3	NI	

31	2-Ethoxy Ethyl Methacrylate	2370-63-0	1.7	NI	1	29.3 ± 5.2	I	I
					2	43.1 ± 5.9	I	
					3	74.4 ± 3.6	NI	
32	hexyl salicylate	6259-76-3	2	NI	1	88.4 ± 8.2	NI	NI
					2	119.5 ± 2.0	NI	
					3	112.2 ± 2.2	NI	
33	Linalyl Acetate	111-95-7	2	NI	1	101.2 ± 1.1	NI	NI
					2	86.8 ± 6.7	NI	
					3	92.6 ± 12.6	NI	
34	terpinyl acetate	80-26-2	2	NI	1	26.2 ± 4.1	I	I
					2	33.6 ± 3.3	I	
					3	36.3 ± 10.9	I	
35	Linalol	78-70-6	2	NI	1	7.9 ± 0.7	I	I
					2	16.6 ± 1.9	I	
					3	25.4 ± 4.0	I	
36	Cinnamaldehyde	104-55-2	2	NI	1	21.4 ± 4.1	I	I
					2	30.1 ± 5.9	I	
					3	35.6 ± 4.6	I	
37	Eugenol	97-53-0	2	NI	1	18.5 ± 2.2	I	I
					2	30.4 ± 4.4	I	
					3	32.2 ± 7.1	I	
38	cyclamen aldehyde	103-95-7	2.3	I	1	30.1 ± 11.2	I	I
					2	24.2 ± 7.7	I	
					3	36.0 ± 4.5	I	
39	1-decanol	112-30-1	2.3	I	1	24.9 ± 3.8	I	I
					2	29.8 ± 6.5	I	
					3	42.1 ± 2.9	I	
40	1-bromohexane	111-25-1	2.7	I	1	36.3 ± 8.2	I	I
					2	40.3 ± 10.8	I	
					3	43.0 ± 3.8	I	
41	alpha-Terpineol	98-55-5	2.7	I	1	13.6 ± 1.3	I	I
					2	17.4 ± 1.6	I	
					3	33.0 ± 5.8	I	
42	1-BromoPentane	110-53-2	2.7	I	1	24.3 ± 15.1	I	I
					2	17.7 ± 3.9	I	
					3	23.7 ± 5.7	I	
43	2-chloromethyl-3,5-dimethyl -4-methoxypyridine HC	86604-75-3	2.7	I	1	10.7 ± 1.5	I	I
					2	11.0 ± 1.7	I	
					3	16.4 ± 2.5	I	
44	butyl methacrylate	97-88-1	3	I	1	28.6 ± 6.1	I	I
					2	24.5 ± 4.1	I	
					3	33.6 ± 11.8	I	
45	di-n-propyl disulphide	629-19-6	3	I	1	74.9 ± 8.6	NI	NI
					2	77.1 ± 8.9	NI	
					3	63.2 ± 7.6	NI	
46	Potassium Hydroxide 5%	1310-58-3	3	I	1	3.3 ± 0.4	I	I
					2	2.5 ± 0.9	I	
					3	3.4 ± 1.4	I	
47	Heptanal	111-71-7	3.3	I	1	13.7 ± 9.9	I	I
					2	18.2 ± 1.8	I	
					3	19.9 ± 2.5	I	
48	benzylmercaptol, 5-(1,1-dimethylethyl)-2-methyl	7340-90-1	3.3	I	1	22.2 ± 8.3	I	I
					2	23.3 ± 2.4	I	
					3	37.2 ± 16.8	I	
49	1-methyl-3-phenyl-1-piperazine	5271-27-2	3.3	I	1	12.1 ± 4.5	I	I
					2	20.5 ± 5.7	I	
					3	13.0 ± 4.4	I	
50	SLS (20% aq)	151-21-3	4	I	1	9.4 ± 0.9	I	I
					2	13.2 ± 1.3	I	
					3	13.4 ± 4.2	I	
51	1,1,1 Trichloroethane	71-55-6	4	I	1	13.4 ± 0.6	I	I
					2	12.0 ± 1.1	I	
					3	10.1 ± 4.3	I	
52	Tetrachloroethylene	127-18-4	4	I	1	11.1 ± 1.3	I	I
					2	17.1 ± 0.9	I	
					3	22.6 ± 2.1	I	
53	Capric acid (decanoic acid)	334-48-5	4	I	1	6.1 ± 2.8	I	I
					2	9.8 ± 0.4	I	
					3	17.6 ± 3.4	I	
54	SLS (5% aq)	127-18-4		I	1	14.5 ± 1.9	I	I
					2	11.4 ± 1.0	I	
					3	14.4 ± 0.9	I	

In vitro/in vivo皮膚刺激性予測の相関

	In vivo classification			
		Irritant	Non-irritant	Total
	In vitro prediction	Irritant	16	11
	Non-irritant	1	26	27
	Total	17	37	54
Sensitivity (%)				94.1
Specificity (%)				70.3
Accuracy (%)				77.8