

Attachment 12a: Cooper statistics on the Silver list, full data in Attachment 2

Number of chemicals tested	67
Number of sensitizers tested	44
Number of sensitizers positive in KeratinoSens	38
Number of sensitizers negative in KeratinoSens	6
Number of non-sensitizers tested	23
Number of non-sensitizers positive in KeratinoSens	4
Number of non-sensitizers negative in KeratinoSens	19
Sensitivity	86.4
Specificity	82.6
Positive predictivity	90.5
Negative predictivity	76.0
False positive rate	17.4
False negative rate	13.6
Accuracy	85.1

False positives

Comments and discussion:

Propylparaben	Known weak human sensitizter from epidemiological studies, but negative in GPMT and LLNA
Ethylvanillin	Contains structural alerts for skin sensitizers (catechol precursor; atromatic aldehyde), but negative in animal and human studies, true false positive
Dimethylisophthalate	Slight induction only at maximal test concentration, borderline but positive with current prediction model
Tween 80	Generally considered non-sensitizer, but positive in guinea pig tests according to Bergh (1). True false positive

False negatives

Benzoyl peroxide	True false-negative, positive in LC-MS assay
Diethylenetriamine	Clear dose response in all repetitions but EC1.5 > 1000 uM, negative in current prediction model
Thioglycerol	Disulfide-bridge forming chemical, positive in LC-MS assay, might be rapidly metabolized in the cells
Resorcinol	Putative prohaptten requiring P450 activation
Eugenol	Putative prohaptten requiring P450 activation
Phenyl benzoate	Acyl transfer agent, rated positive in LC-MS based peptide reactivity assay, probably due to reaction with amine groups

¹ Bergh, M.,Magnusson, K.,Nilsson, J. L.and Karlberg, A. T., (1997) Contact allergenic activity of Tween 80 before and after air exposure. Contact Dermatitis 37, 9-18.