

Alépée et al.:

Development of a Defined Approach for Eye Hazard Identification of Solid Chemicals According to the Three UN GHS Categories

Supplementary Data

Tab. S2: Performance of the DAS in the bottom-up approach for the training set (N = 71) and test set (N = 38)

UN GHS	Prediction DAS – Training set		
	Cat. 1	Cat. 2	No Cat.
Cat. 1 (N = 20)	75.0%	25.0%	0.0%
Cat. 2 (N = 12)	27.7%	53.4%	18.9%
No Cat. (N = 39)	0.0%	30.8%	69.2%

UN GHS	Prediction DAS – Test set		
	Cat. 1	Cat. 2	No Cat.
Cat. 1 (N = 11)	81.8%	18.2%	0.0%
Cat. 2 (N = 6)	33.3%	50.0%	16.7%
No Cat. (N = 21)	4.8%	23.8%	71.4%

Tab. S3: Performance of the DAS and SkinEthic™ HCE TTT compared to the UN GHS classification based on the Draize eye test and concordance in prediction between both NAMs for the same set of solids (N = 72)

UN GHS	NAM	Prediction			Concordance
		Cat. 1	Cat. 2	No Cat.	
Cat. 1 (N = 24)	DAS	79.2%	20.8%	0.0%	83.3%
	TTT	82.0%	18.0%	0.0%	
Cat. 2 (N = 16)	DAS	31.3%	50.6%	18.2%	62.5%
	TTT	18.8%	53.2%	28.0%	
No Cat. (N = 32)	DAS	3.1%	32.6%	67.4%	81.3%
	TTT	3.1%	26.0%	70.8%	