

Natsch:

# Integrated Skin Sensitization Assessment Based on OECD Methods (III): Adding Human Data to the Potency Assessment

## Supplementary Data

### Combination of KS and h-CLAT data on the different datasets and for the different endpoints

The combination of h-CLAT and KS data without reactivity data led to EQ6 in the published models. This equation may be useful for a conservative assessment of chemicals that are only positive in these two assays but negative in the reactivity assay.

This equation was recalculated for all three data subsets and for the different *in vivo* targets. As shown in Table S1, in all cases an increase of the weight of KS EC1.5 and h-CLAT MIT along with a drop in cytotoxicity coefficients was noted, confirming the analysis on the other combinations of input parameters (EQ1, EQ4 and EQ5).

**Tab. S1: Regression coefficients and statistics for predictive models trained on the RCPL**

Model	Dataset	Constant	EC1.5	IC50	MIT	CV75	VP <sub>norm</sub>	R <sup>2</sup>	N	EQ
<b>EQ6 pEC3</b>	ALTEX publication	0.09	0.22	0.06	0.28	0.34	-0.12	52%	188	EQ6
vs. pEC3	Published PV	-0.44	<b>0.34</b>	<b>-0.08</b>	<b>0.21</b>	<b>0.70</b>	-0.21	74%	31	EQ6a
vs. pPV	Published PV	-0.56	<b>0.56</b>	<b>-0.35</b>	<b>0.48</b>	<b>0.34</b>	0.24	70%	31	EQ6b
vs. pEC3	Extended PV	0.08	<b>0.24</b>	<b>0.07</b>	<b>0.37</b>	<b>0.23</b>	-0.07	56%	139	EQ6c
vs. pPV	Extended PV	0.17	<b>0.42</b>	<b>-0.196</b>	<b>0.50</b>	<b>0.04</b>	-0.02	53%	139	EQ6d
vs. pEC3	Human data set	0.06	<b>0.23</b>	<b>0.38</b>	<b>0.26</b>	<b>0.03</b>	0.015	57%	62	EQ6e
vs. pPV	Human data set	0.29	<b>0.46</b>	<b>-0.11</b>	<b>0.36</b>	<b>-0.05</b>	0.012	49%	62	EQ6f
Vs. pDSA04	Human data set	0.32	<b>0.46</b>	<b>-0.057</b>	<b>0.354</b>	<b>-0.148</b>	0.02	44%	62	EQ6g