**Table S4a.** Substances misclassified by best performing models for LLNA using Strategy B

|  |  |  |  |
| --- | --- | --- | --- |
| **Chemical Name** | **Predicted LLNA Category** | **Reference****LLNA****Categorya** | **LLNA EC3** |
| Isoeugenolb | 1B | 1A | 1.33 |
| Formaldehyde | 1B | 1A | 1.43 |
| 2-Mercaptobenzothiazolec | 1A | 1B | 2.27 |
| Methyl 2-nonynoate | 1A | 1B | 2.50 |
| Diethyl maleate | 1A | 1B | 3.41 |
| Benzylidene acetone | 1A | 1B | 3.70 |
| 1,2-Benzisothiazolin-3-one | 1A | 1B | 7.10 |
| Perillaldehyde | 1A | 1B | 8.10 |
| 2,3-Butanedione | 1A | 1B | 11.00 |
| Butyl acrylate | 1A | 1B | 16.38 |
|  |  |  |  |
| Phthalic anhydrided | Nonsensitizer | 1A | 0.36 |
| Coumarind | Nonsensitizer | 1B | 29.62 |
| Nonanoic acidd | Nonsensitizer | 1B | 35.00 |
| Anilined | Sensitizer | Nonsensitizer | 31.45 |

**Table S4b.** Substances misclassified by best performing models for human using Strategy B

|  |  |  |  |
| --- | --- | --- | --- |
| **Chemical Name** | **Predicted Human Category** | **Reference Human Categorye** | **Basketter *et al.* (2014) Categoryf** |
| 3 and 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexane-1-carboxaldehyde [Lyral HMPCC] | 1B | 1A | 2 |
| 3-Dimethylaminopropylaminec | 1B | 1A | 2 |
| Formaldehyde | 1B | 1A | 2 |
| Isoeugenolb | 1B | 1A | 2 |
| Bisphenol A-diglycidyl ether | 1A | 1B | 3 |
| Butyl glycidyl ether | 1A | 1B | 3 |
| Citral | 1A | 1B | 3 |
| 1,4-Dihydroquinoneb | 1A | 1B | 3 |
| 2-Hydroxyethyl acrylate | 1A | 1B | 3 |
| 2-Mercaptobenzothiazolec | 1A | 1B | 3 |
| Tetramethylthiuram disulfide | 1A | 1B | 3 |
|  |  |  |  |
| Benzocained | Nonsensitizer | 1B | 4 |
| Coumarind | Nonsensitizer | 1B | 3 |
| Penicillin Gd | Nonsensitizer | 1B | 3 |
| Sulfanilamided | Nonsensitizer | 1B |  |
| 2-Methoxy-4-methylphenold | Sensitizer | Nonsensitizer |  |
| Pentachlorophenold | Sensitizer | Nonsensitizer | 5 |

EC3, estimated test substance concentration that produces a stimulation index of 3, the threshold for a substance to be considered a sensitizer in the LLNA; DSA05, induction dose per skin area (µg/cm2) that produces a 5% response in the test population; LLNA, murine local lymph node assay

a The LLNA data set contained 35 1A, and 52 1B sensitizers.

b Prehapten.

c Prohapten.

d Misclassifications from Tier 1.

e The human data set contained 26 1A and 31 1B sensitizers.

f Potency categories 1 and 2 correspond to GHS 1A and potency categories 3 and 4 correspond to GHS 1B (Basketter *et al.,* 2014).