**Table S3.** Tier Two binary classification of strong vs. weak sensitizersa for Strategy B

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **LLNA/**  **Humanb** | **Variable Setc** | **Data**  **Set** | **True Positive** | **False Negative** | **Sensitivity (1A %)** | **True Negative** | **False Positive** | **Specificity (1B %)** | **Accuracy (%)** |
|  |  | Training | 25 | 3 | 89 ± 12 | 35 | 5 | 88 ± 10 | 88 ± 8 |
|  | III | Test | 6 | 1 | 86 ± 26 | 11 | 1 | 92 ± 15 | 89 ± 14 |
| LLNA |  | LOOCV | 32 | 3 | 91 ± 9 | 44 | 8 | 85 ± 10 | 87 ± 7 |
|  |  | Training | 26 | 2 | 93 ± 9 | 32 | 8 | 80 ± 12 | 85 ± 9 |
|  | IV | Test | 6 | 1 | 86 ± 26 | 9 | 3 | 75 ± 25 | 79 ± 18 |
|  |  | LOOCV | 32 | 3 | 91 ± 9 | 41 | 11 | 79 ± 11 | 84 ± 8 |
|  |  |  |  |  |  |  |  |  |  |
|  |  | Training | 17 | 2 | 90 ± 14 | 17 | 5 | 77 ± 18 | 83 ± 11 |
|  | III | Test | 6 | 1 | 86 ± 26 | 7 | 2 | 78 ± 27 | 81 ± 19 |
| Human |  | LOOCV | 22 | 4 | 85 ± 14 | 24 | 7 | 77 ± 15 | 81 ± 10 |
|  |  | Training | 17 | 2 | 90 ± 14 | 16 | 6 | 73 ± 19 | 81 ± 12 |
|  | IV | Test | 6 | 1 | 86 ± 26 | 7 | 2 | 78 ± 27 | 81 ± 19 |
|  |  | LOOCV | 22 | 4 | 85 ± 14 | 23 | 8 | 74 ± 15 | 79 ± 11 |

LLNA, murine local lymph node assay; LOOCV, leave-one-out cross-validation; SVM, support vector machine.

The values after ± indicate 95% confidence limits of proportion for correct classification rate.

a Table summarizes performance of models using the SVM machine learning approach in classification of 1A (strong) and 1B (weak) sensitizers according to the Globally Harmonized System of Classification and Labeling of Chemicals (UN 2015).

b The LLNA data set contained 87 sensitizers: 35 1A and 52 1B. The human data set contained 57 sensitizers: 26 1A and 31 1B.

c Variable sets are defined in Table 4.