**Table S2.** Strategy A model performance for the test set classificationa

|  |  |  |  |
| --- | --- | --- | --- |
| **LLNA/Humanb** | **Models** | **Variable set** | **Overall accuracy (%)** |
|  |  | I | 58 |
|  | CART | II | 46 |
|  |  | III | 65 |
|  |  | IV | 54 |
|  |  | I | 65 |
|  | LDA | II | 46 |
|  |  | III | 58 |
| LLNA |  | IV | 65 |
|  |  | I | 62 |
|  | LR | II | 58 |
|  |  | III | 64 |
|  |  | IV | 62 |
|  |  | I | 65 |
|  | SVM | II | 75 |
|  |  | III | 77 |
|  |  | IV | 69 |
|  |  |  |  |
|  |  | I | 58 |
|  | CART | II | 42 |
|  |  | III | 58 |
|  |  | IV | 58 |
|  |  | I | 67 |
|  | LDA | II | 42 |
|  |  | III | 54 |
| Human |  | IV | 63 |
|  |  | I | 58 |
|  | LR | II | 42 |
|  |  | III | 62 |
|  |  | IV | 58 |
|  |  | I | 67 |
|  | SVM | II | 46 |
|  |  | III | 71 |
|  |  | IV | 71 |

CART, classification and regression tree; LDA, linear discriminant analysis; LR, logistic regression; LLNA, murine local lymph node assay; SVM, support vector machine.

a Strategy A modeled all three categories of response simultaneously.

b The LLNA data set contained 120 substances: 35 strong sensitizers, 52 weak sensitizers, and 33 nonsensitizers. The human data set contained 87 substances: 26 strong sensitizers, 31 weak sensitizers, and 30 non sensitizers.