Supplemental Information

Presented below are the confusion matrices used to create Tables 3 & 4, which correspond to the 0.5 and 1.0 mean intensity cut-offs, respectively. These consist of training and test sets created by independently removing 2 spectra from each class and using the remaining data as the training set. For Tables S1a and S2a, the 5th and 6th item of each class was removed. Similarly, for Tables S1b and S2b, the 4th and 7th item of each class was removed. For Tables S1c and S2c, the 3rd and 8th item from each class was removed. It should be noted that end values in each set were not removed, to ensure training and test sets were not created by disproportionately sampling from any given class, as each class did not have the same number of items (Table 1). For the 0.5 mean intensity cut-off (Table 3), the values presented in Tables S1a, S1b, and S1c were averaged. Likewise, for the 1.0 mean intensity cut-off (Table 4), the values presented in Tables S2a, S2b, and S2c were averaged. As described in the main text, each cell of each confusion matrix consists of three values, the calibration set/cross-validation set/test set, where periods ('.') denote a value of '0' for readability. A matrix with a diagonal matching the values shown in the column titled 'N=' indicate a model with 100% classification success. An example of an imperfect model would be that of Table S1a, row 'True 2,' where there are 6 correct cross-validations, where one of the missed cross-validations was identified as class 7 and one was classified as class 9. Additionally, in the 'True 2' column, there was one miss-classification in the validation set, which was attributed to class 9. It can be seen amongst all data presented below that the classification rates were high with no more than 0 calibration set miss-classifications, 6 cross-validation set miss-classifications, or 1 test set miss-classification for any given model.

Table S1a. Confusion Matrix for PLS-DA applied to 0.5 Cut-off Filtered LIBS Data (5,6)
Values of '0' are replaced in the table with '.' for clarity of reading.

	N =	Pred. 1	Pred. 2	Pred. 3	Pred. 4	Pred. 5	Pred. 6	Pred. 7	Pred. 8	Pred. 9
True 1	8/8/2	8/6/2	. /. /.	. /. /.	. /1/.	. /. /.	. /1/.	. /. /.	. /. /.	. /. /.
True 2	8/8/2	. /. /.	8/6/1	. /. /.	. /. /.	. /. /.	. /. /.	. /1/.	. /. /.	. /1/1
True 3	8/8/2	. /. /.	. /. /.	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.
True 4	8/8/2	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.
True 5	9/9/2	. /. /.	. /. /.	. /. /.	. /. /.	9/9/2	. /. /.	. /. /.	. /. /.	. /. /.
True 6	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.	. /. /.	. /. /.
True 7	7/7/2	. /. /.	. /1/.	. /. /.	. /. /.	. /. /.	. /. /.	7/6/2	. /. /.	. /. /.
True 8	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.
True 9	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2

Table S1b. Confusion Matrix for PLS-DA applied to 0.5 Cut-off Filtered LIBS Data (4,7)
Values of '0' are replaced in the table with '.' for clarity of reading.

	N =	Pred. 1	Pred. 2	Pred. 3	Pred. 4	Pred. 5	Pred. 6	Pred. 7	Pred. 8	Pred. 9
True 1	8/8/2	8/4/2	. /. /.	. /. /.	. /./.	. /. /.	. /4/.	. /. /.	. /. /.	. /. /.
True 2	8/8/2	. /. /.	8/6/2	. /. /.	. /. /.	. /. /.	. /. /.	. /1/.	. /. /.	. /1/.
True 3	8/8/2	. /. /.	. /. /.	8/8/1	. /. /.	. /. /.	. /. /.	. /. /1	. /. /.	. /. /.
True 4	8/8/2	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.
True 5	9/9/2	. /. /.	. /. /.	. /1 /.	. /. /.	9/8/2	. /. /.	. /. /.	. /. /.	. /. /.
True 6	8/8/2	. /. /.	. /. /.	. /. /.	. /1 /.	. /. /.	8/7/2	. /. /.	. /. /.	. /. /.
True 7	7/7/2	. /. /.	. /./.	. /. /.	. /. /.	. /. /.	. /. /.	7/7/2	. /. /.	. /. /.
True 8	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.
True 9	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2

Table S1c. Confusion Matrix for PLS-DA applied to 0.5 Cut-off Filtered LIBS Data (3,8)
Values of '0' are replaced in the table with '.' for clarity of reading.

N =	Pred. 1	Pred. 2	Pred. 3	Pred. 4	Pred. 5	Pred. 6	Pred. 7	Pred. 8	Pred. 9
8/8/2	8/7/2	. /. /.	. /. /.	. /./.	. /. /.	. /1/.	. /. /.	. /. /.	. /. /.
8/8/2	. /. /.	8/6/2	. /. /.	. /. /.	. /. /.	. /. /.	. /1/.	. /. /.	. /1/.
8/8/2	. /. /.	. /. /.	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.
8/8/2	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.
9/9/2	. /. /.	. /. /.	. /1 /.	. /. /.	9/7/2	. /1 /.	. /. /.	. /. /.	. /. /.
8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.	. /. /.	. /. /.
7/7/2	. /. /.	. /./.	. /. /.	. /. /.	. /. /.	. /. /.	7/7/2	. /. /.	. /. /.
8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.
8/8/2	. /. /.	. /1 /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/7/2

Table S2a. Confusion Matrix for PLS-DA applied to 1.0 Cut-off Filtered LIBS Data (5,6)
Values of '0' are replaced in the table with '.' for clarity of reading.

	N =	Pred. 1	Pred. 2	Pred. 3	Pred. 4	Pred. 5	Pred. 6	Pred. 7	Pred. 8	Pred. 9
True 1	8/8/2	8/5/2	. /. /.	. /. /.	. /1/.	. /. /.	. /2/.	. /. /.	. /. /.	. /. /.
True 2	8/8/2	. /. /.	8/8/1	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /1
True 3	8/8/2	. /. /.	. /. /.	8/7/2	. /. /.	. /1 /.	. /. /.	. /. /.	. /. /.	. /. /.
True 4	8/8/2	. /1 /.	. /. /.	. /. /.	8/7/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.
True 5	9/9/2	. /. /.	. /. /.	. /. /.	. /. /.	9/9/2	. /. /.	. /. /.	. /. /.	. /. /.
True 6	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.	. /. /.	. /. /.
True 7	7/7/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	7/7/2	. /. /.	. /. /.
True 8	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.
True 9	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2

Table S2b. Confusion Matrix for PLS-DA applied to 1.0 Cut-off Filtered LIBS Data (4,7)
Values of '0' are replaced in the table with '.' for clarity of reading.

	N =	Pred. 1	Pred. 2	Pred. 3	Pred. 4	Pred. 5	Pred. 6	Pred. 7	Pred. 8	Pred. 9
True 1	8/8/2	8/8/2	. /. /.	. /. /.	. /./.	. /. /.	. /./.	. /. /.	. /. /.	. /. /.
True 2	8/8/2	. /. /.	8/6/2	. /. /.	. /. /.	. /. /.	. /. /.	. /./.	. /. /.	. /2/.
True 3	8/8/2	. /. /.	. /. /.	8/7/2	. /. /.	. /1 /.	. /. /.	. /. /.	. /. /.	. /. /.
True 4	8/8/2	. /.1/.	. /. /.	. /. /.	8/5/2	. /. /.	. /2 /.	. /. /.	. /. /.	. /. /.
True 5	9/9/2	. /. /.	. /. /.	. /. /.	. /. /.	9/9/2	. /. /.	. /. /.	. /. /.	. /. /.
True 6	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.	. /. /.	. /. /.
True 7	7/7/2	. /. /.	. /./.	. /. /.	. /. /.	. /. /.	. /. /.	7/7/2	. /. /.	. /. /.
True 8	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /1 /.	8/7/2	. /. /.
True 9	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2

Table S2c. Confusion Matrix for PLS-DA applied to 1.0 Cut-off Filtered LIBS Data (3,8)
Values of '0' are replaced in the table with '.' for clarity of reading.

	N =	Pred. 1	Pred. 2	Pred. 3	Pred. 4	Pred. 5	Pred. 6	Pred. 7	Pred. 8	Pred. 9
True 1	8/8/2	8/8/2	. /. /.	. /. /.	. /./.	. /. /.	. /./.	. /. /.	. /. /.	. /. /.
True 2	8/8/2	. /. /.	8/7/2	. /. /.	. /. /.	. /. /.	. /. /.	. /./.	. /. /.	. /1/.
True 3	8/8/2	. /. /.	. /. /.	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.
True 4	8/8/2	. /1 /.	. /. /.	. /. /.	8/7/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.
True 5	9/9/2	. /. /.	. /. /.	. /1 /.	. /. /.	9/8/2	. /. /.	. /. /.	. /. /.	. /. /.
True 6	8/8/2	. /. /.	. /. /.	. /. /.	. /1 /.	. /. /.	8/7/2	. /. /.	. /. /.	. /. /.
True 7	7/7/2	. /. /.	. /./.	. /. /.	. /. /.	. /. /.	. /. /.	7/7/2	. /. /.	. /. /.
True 8	8/8/2	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/8/2	. /. /.
True 9	8/8/2	. /. /.	. /1 /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	. /. /.	8/7/2