Article

Rapid Detection of Single- and Co-contaminant Aflatoxins and Fumonisins in Ground Maize using Hyperspectral Imaging Techniques

Yong-Kyoung Kim [1], Insuck Baek [2], Kyung-Min Lee [3], Geonwoo Kim [2,4], Seyeon Kim [1], Sung-Youn Kim [1], Diane Chan [2], Timothy J. Herrman [3], Namkuk Kim [1,*] and Moon S. Kim [2,*]

[1] Division of Safety Analysis, Experiment & Research Institute, National Agricultural Products Quality Management Service, Gimcheon 39660, Republic of Korea; ykkim79@korea.kr (Y.-K.K.); syesther1114@korea.kr (S.K.) youn5326@korea.kr (S.-Y.K.)

[2] Environmental Microbial and Food Safety Laboratory, Agricultural Research Service, U.S. Department of Agriculture, Powder Mill Rd., Building 303 BARC-East, Beltsville, MD 20705, USA; insuck.baek@usda.gov (I.B.); geonwookim@gnu.ac.kr (G.K.); diane.chan@usda.gov (D.C.)

[3] Office of the Texas State Chemist, Texas A&M AgriLife Research, Texas A&M University System, College Station, TX 77841, USA; kml@otsc.tamu.edu (K.-M.L.); tjh@otsc.tamu.edu (T.J.H.)

[4] Department of Bio-industrial Machinery Engineering, College of Agriculture and Life Science, Gyeongsang National University, 501 Jinju-daero, Jinju-si 52828, Republic of Korea

* Correspondence: nkvirus@korea.kr (N.K.); moon.kim@usda.gov (M.S.K.); Tel.: +82-54-429-7766 (N.K.); +1-301-504-8462 (M.S.K.)

Table S1. Chemometrics results of the PLS-DA and SVM model for mycotoxin-contaminated samples analyzed by Fluorescence combined with different preprocessing methods.

Preprocessing Method	PLS-DA					SVM				
	Calibration (%)	Validation (%)				Calibration (%)	Validation (%)			
	Accuracy	Accuracy	Precision	Recall	F1 score	Accuracy	Accuracy	Precision	Recall	F1 score
Raw	52.2	32.6	48.6	32.6	34.9	50.5	39.1	29.1	40.9	29.6
Max	58.3	39.1	52.8	39.4	41.3	92.9	80.4	81.1	80.1	80.0
Mean	57.7	37.0	51.3	37.1	39.5	95.1	26.1	6.5	25.0	10.3
Range	57.7	37.0	46.6	37.3	39.1	92.9	87.0	87.1	86.6	86.2
SNV	39.2	32.6	41.7	32.6	28.0	97.3	89.1	90.2	88.6	88.7
MSC	39.0	32.6	41.7	32.6	28.0	50.5	26.1	6.5	25.0	10.3
Smoothing	51.6	30.4	44.5	30.3	32.0	50.5	41.3	32.2	43.2	32.3
SG1	42.3	32.6	39.3	32.2	30.3	50.5	37.0	26.2	38.6	27.9
SG2	43.7	34.8	40.6	34.5	32.0	100	67.4	71.7	67.6	67.9

*Precision, Recall, F1 scores are average value of each groups.

Table S2. Chemometrics results of the PLS-DA, SVM model for mycotoxin-contaminated samples analyzed by VNIR combined with different preprocessing methods.

Preprocessing Method	PLS-DA					SVM				
	Calibration (%)	Validation (%)				Calibration (%)	Validation (%)			
	Accuracy	Accuracy	Precision	Recall	F1 score	Accuracy	Accuracy	Precision	Recall	F1 score
Raw	31.3	28.3	38.6	28.4	21.4	87.9	63.0	62.5	63.1	62.7
Max	30.2	23.9	12.3	24.1	16.1	85.9	71.7	71.2	71.4	71.1
Mean	29.7	23.9	12.0	24.1	15.9	100	26.1	6.5	25.0	10.3
Range	28.6	21.7	11.0	22.0	14.6	81.3	71.7	72.6	71.6	71.9
SNV	20.3	19.6	9.2	20.1	12.2	99.5	67.4	67.7	67.0	67.1
MSC	24.7	23.9	23.9	24.2	18.6	99.5	26.1	6.5	25.0	10.3
Smoothing	31.3	30.4	39.7	30.7	22.8	90.1	60.9	61.7	61.0	61.1
SG1	29.1	26.1	13.0	26.3	17.3	100	50.0	47.9	49.2	48.4

SG2	28.6	34.8	40.6	34.5	32.0	79.1	67.4	71.7	67.6	67.9

Table S3. Chemometrics results of the PLS-DA, SVM model for mycotoxin-contaminated samples analyzed by SWIR combined with different preprocessing methods.

Preprocessing Method	PLS-DA						SVM			
	Calibration (%)	Validation (%)				Calibration (%)	Validation (%)			
	Accuracy	Accuracy	Precision	Recall	F1 score	Accuracy	Accuracy	Precision	Recall	F1 score
Raw	58.2	56.5	65.1	56.4	57.3	97.8	89.1	90.8	88.8	89.0
Max	58.8	60.9	77.0	60.6	57.4	91.8	95.7	96.2	95.8	95.6
Mean	53.3	58.7	68.9	58.5	58.2	26.1	26.1	6.5	25.0	10.3
Range	54.9	50.0	63.9	49.8	49.9	87.4	87.0	91.2	86.7	86.8
SNV	59.9	54.3	66.8	54.2	53.3	100	91.3	92.1	91.3	91.5
MSC	57.1	54.3	66.8	54.2	53.3	100	23.9	6.0	25.0	9.6
Smoothing	59.9	52.2	60.1	52.1	52.5	96.7	89.1	90.8	88.8	89.0
SG1	59.3	47.8	61.7	47.5	50.4	100	95.7	95.8	95.6	95.6
SG2	59.9	34.8	40.6	34.5	32.0	98.4	67.4	71.7	67.6	67.9