

Determination of Fatty Acid Composition in Soybean Seed, Using Near Infrared Reflectance Spectroscopy

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Objectives :

The objectives of this study were to determine the potential use of near infrared reflectance spectroscopy(NIRS) for fatty acid analysis in soybean seed, and to provide the efficient mass screening technique for selection of high quality soybean.

Materials and Methods :

Materials : 259 accessions (ground soybean seed samples)

Fatty acid analysis : GC-FID(Column: HP-FFAP, Methylation: H₂SO₄-MeOH) method

Scanning of NIRS spectra : NIRSystem 6500 monochrometer(400 - 2500nm)

Calibration and Validation : Using the WinISI program(ver. 1.52)

Results and Discussion :

The seed oil of common soybean consists of approximately 11, 4, 24, 54, and 7% for palmitic, stearic, oleic, linoleic, and linolenic acid, respectively. Likely many other oils of plant origin, most fatty acids in soybean are unsaturated. Considerable research has centered around seed oil quality and its relationship with these fatty acids. However, little research has looked at using NIRS for fatty acid analysis in soybean seed.

The NIRS fatty acid equations had low standard error of calibration (SEC) values for all five fatty acids, and moderate R^2 values for three of the five fatty acids. Additionally, the predicted means for each fatty acids were similar to the means based on the GC analysis. These data suggest that the oleic, linoleic, and linolenic acid NIRS equation have potential use as a crude screening method for fatty acid composition in soybean seed. The palmitic and stearic acid equations had moderate SEC values, but much lower R^2 values than the other three fatty acid equations, which may be due to the low standard deviation.

Based on the bias, standard error of prediction(SEP), and R^2 statistics, the NIRS fatty acid equations accurately predicted oleic, linoleic, and linolenic acid composition of the validation set. These statistics indicate that three of the five fatty acids can be estimated in soybean samples using NIRS with good accuracy.

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This research is supported by Biogreen 21, RDA.

Table 1. Gas chromatography laboratory reference value statistics for five fatty acids based on 194 soybean calibration sample set.

Parameter	Low(%)	High(%)	Mean(%)	SD(%)
Palmitic acid	8.85	14.14	11.27	0.88
Stearic acid	2.24	4.73	3.18	0.48
Oleic acid	15.08	48.15	26.19	6.77
Linoleic acid	30.47	60.22	51.69	5.54
Linolenic acid	4.43	10.72	7.65	1.28

Table 2. Gas chromatography laboratory reference value statistics for five fatty acids based on 65 soybean validation sample set.

Parameter	Low(%)	High(%)	Mean(%)	SD(%)
Palmitic acid	9.04	13.09	11.46	0.89
Stearic acid	2.28	4.79	3.43	0.50
Oleic acid	15.10	40.20	24.86	5.83
Linoleic acid	40.71	60.20	52.70	4.57
Linolenic acid	5.46	9.61	7.55	1.06

Table 3. Near infrared spectroscopy(NIRS) calibration equation statistics for five fatty acids.

Fatty acid	Math	Regression	Term	Scatter	R^2	SEC
Oleic acid	2, 8, 6, 1	Stepwise-MLR	9	SNVD	0.974(n=188)	0.993
Linoleic acid	2, 8, 6, 1	Stepwise-MLR	8	SNVD	0.967(n=179)	0.910
Linolenic acid	2, 8, 6, 1	Stepwise-MLR	9	SNVD	0.884(n=184)	0.375
Palmitic acid	1, 4, 4, 1	Stepwise-MLR	7	SNVD	0.541(n=188)	0.553
Stearic acid	2, 8, 6, 1	Stepwise-MLR	7	SNVD	0.557(n=182)	0.290

Table 4. The performance of the initial five fatty acid calibrations based on validation statistics from a new set of 65 soybean samples.

Fatty acid	SEP	R^2	Bias	R. SD(%)	SEP/M(%)
Oleic acid	0.992	0.971	0.056	1.00	0.04
Linoleic acid	1.025	0.950	0.066	0.91	0.02
Linolenic acid	0.408	0.851	-0.034	0.41	0.05
Palmitic acid	0.591	0.582	-0.142	0.58	0.05
Stearic acid	0.411	0.339	0.031	0.41	0.13