Predicting Oxidative Stability of Vegetable Oils Using Neural Network System and Endogenous Oil Components

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ABSTRACT: The usefulness of Artificial Neural Network Systems (ANNW) to predict the stability of vegetable oil based on chemical composition was evaluated. The training set, comprised of a composition of major and minor components of vegetable oil as inputs and as outputs, induction period and values of slopes for initiation and propagation, was measured by oxygen consumption. The best predictability was achieved for oils stored at 35°C with light exposure, when the major fatty acids, chlorophylls, tocopherols, tocotrienols, and metals were used as predictors. For oils stored at 65°C without light, a good predictability was obtained when composition of the major fatty acids and the amounts of tocopherols and tocotrienols were used. These results suggest that vegetable oil stability can be successfully predicted by ANNW when partial oil composition is known.

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KEY WORDS: Artificial neutral network, fatty acids, oxidative stability, prediction, sterols, tocopherols, tocotrienols, vegetable oils.

Lipid oxidation leads to rancidity, and it is the decisive factor determining the shelf life of food products, even when the fat content is low. A substantive amount of work has been conducted to better understand the mechanism of oxidation of polyunsaturated fatty acids, antioxidants action, and the effect of decomposition products of oxidized lipids on the formation of off-flavors. Oxidative stability of vegetable oil is a function of the presence of unsaturated fatty acids, oxygen, endogenous minor components, and conditions of storage (1).

Neural Networks is a data-processing technique simulating human brain analytical functions, which has the ability to learn by experience (2). This system is useful when no exact mathematical relationship is available and also to solve linear and nonlinear prediction problems (3–5). Artificial Neural Network Systems (ANNW) are usually composed of computer-simulated layers of processing elements known as artificial neurons (6). Those neurons receive input signals and pass them to the hidden layers through a set of weighted connections. Each neuron can process a piece of information at the same time as other units do. The processing of information occurs in parallel and is distributed throughout each unit composing the network. The neuron transfers the weighted sum through a sigmoidal function that compresses a wide domain of inputs into a limited range of outputs (1,5,7). During the training phase of the ANNW, the predicted output of the system is subsequently compared with the actual output, and the weights of connection between the processing units are modified to minimize the deviations. This is accomplished by a feed-forward layered structure, where each unit in a given layer is fully connected to every unit in the succeeding layer. This structure includes the forward propagation of neuron activation and the backward propagation of the error, with concomitant adjustments to the connections' weights. In this back-propagation algorithm concept, the ANNW continues to make changes to internal connections by a trial-and-error process until a defined accuracy has been achieved (3,5,8,9). Once the system has been trained by a set of training facts (inputs and outputs), a new set of inputs can be presented and the ANNW will predict the corresponding value of outputs (2,10). Borggaard and Thodberg (4) demonstrated that ANNW are able to predict well, based on new observations (inputs and outputs) even if they fall outside the range of the training set.

Recently, Artificial Neural Networks have been successfully applied in many areas of food quality assessment. Goodacre and Kell (11,12) assessed the adulteration of olive oils using pyrolysis mass spectra of oils and ANNW. Zhang *et al.* (13) presented ANNW models for predicting the secondary structure of globular proteins. Arteaga and Nakai (6) applied neural network and physicochemical properties of food-related proteins to predict foam capacity and stability, and the emulsion activity index. These authors reported that ANNW had better prediction ability than Principal Component Regression (PCR). Horimoto *et al.* (14) used ANNW with several variables to predict the volume of bread loafs made from different wheat cultivars. Vallejo-Cordoba *et al.* (9) used a Neural Network system to predict milk shelf life applying multivariate interpretation of gas chromatographic profiles of flavor components and sensory data. These authors

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reported that ANNW were better able to predict shelf life than PCR. Ruan *et al.* (8) showed high predictability of the rheological properties of dough from the torque developed during mixing using ANNW.

The application of ANNW to predict oxidative stability of oils based on their composition is lacking. The main objective of this work was to evaluate the ability of ANNW to predict vegetable oil oxidative stability utilizing composition and content of endogenous oil components.

MATERIALS AND METHODS

Composition of the oils. Thirty-three vegetable oils were used in this study, including standard and genetically modified varieties of many oils. These included BOR, borage, cold-pressed; CAO, regular canola, refined, bleached, and deodorized (RBD), produced from third-grade seeds; CAN, regular canola, RBD; CAS, regular canola, RBD; CAR, low-linolenic canola, RBD; CHO, high-oleic canola, RBD; COL, high-oleic low-linolenic canola, RBD; COR, corn, RBD; CRN, corn, RBD; CRW, corn, RBD; COC, coconut, pressed and refined; CTO, cottonseed, RBD; COT, cottonseed, RBD; EPR, evening primrose, cold-pressed; FCO, regular flax, cold-pressed; FLL, low-linolenic flax, RBD; OEV, virgin olive, cold-pressed; OPR, olive pomace, RBD; ORF, olive, RBD; PAL, palm, refined; PLG, red palm, refined; PLK, palm kernel, refined; PEA, peanut, RBD; PNT, peanut, RBD and RIO, rice bran, RBD; RBO, rice bran, RBD; RWO, rice bran, RBD and winterized; SUN, regular sunflower, RBD; SUR, regular sunflower, RBD; SHO, high-oleic sunflower, RBD; SOY, soybean, RBD; SYS, soybean, RBD; SYB, soybean, RBD. The same oils with different symbols indicate different processors.

Selected oils were analyzed for fatty acid composition (AOCS Ce 1-62)(15), free fatty acids (AOCS Ca 5a-40)(15), neutral lipids, phospholipids, glycolipids (16), tocopherols and tocotrienols (17), sterols (18), chlorophyll (AOCS Cd 13d-55)(15), carotenoids (19), metals (AOCS Cd 18-79)(15), phenolic acids (20,21), and triglycerides (22).

Oxygen consumption. The oxidative stability of oils was evaluated by measurement of oxygen consumption during accelerated storage using the modified procedure described by Jung *et al.* (23,24). Briefly, samples of 10 mL of oil were placed in 60-mL serological bottles, providing a ratio of surface area to volume equal to one. Air-tight sealed bottles with oils were stored in the presence and absence of light at 35 and at 65°C, respectively. Oxygen content in the head space was measured every 12 h for a period of 14 d by injecting 20 μL of gases in duplicate. Permanent gases were separated on a column with molecular sieve packing 5A (1.25 mm × 2 m, 80/100 mesh, Supelco, Bellefonte, PA) using hydrogen as a carrier gas and a thermal conductivity detector. Figures 1 and 2 present typical oxygen consumption curves for oils stored with and without light exposure, respectively.

Artificial Neural Networks. For all analysis software, BrainMaker (California Scientific Software, Nevada City, CA) was used. The oils were separated into two sets, one set was used as training data, while the other was used to predict values. About half of the analyzed 33 oils were assigned to train the program, while the other oils were used to predict the values related to their stability. The oil composition was used as input data (predictors), while the values of induction periods (ip), slopes of initiation (k_1), and slopes of propagation (k_2), obtained from oxygen uptake measurements, served as outputs.

The ANNW software was trained using the standard back-propagation algorithm and automatically tested after each 20 runs during the training. The training was stopped when the squared error reached a value of 0.05. The number of hidden neurons was initially determined by the relation: (inputs + outputs)/2 (25). During training, software was set up to automatically prune neurons after each training section. The learning and smoothing rates were set between 0.08 and 0.1, while the training tolerance was set at 0.1. Correlation coefficients (r^2) and standard error of the estimate (SEE) were calculated between predicted and experimental values.

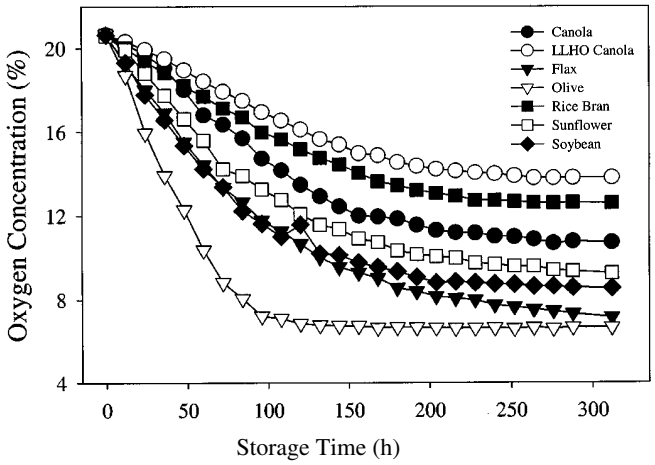

FIG. 1. Consumption of oxygen by selected oils during storage at 35°C with light presence. For description see Materials and Methods section. LLHO, low-linolenic high-oleic.

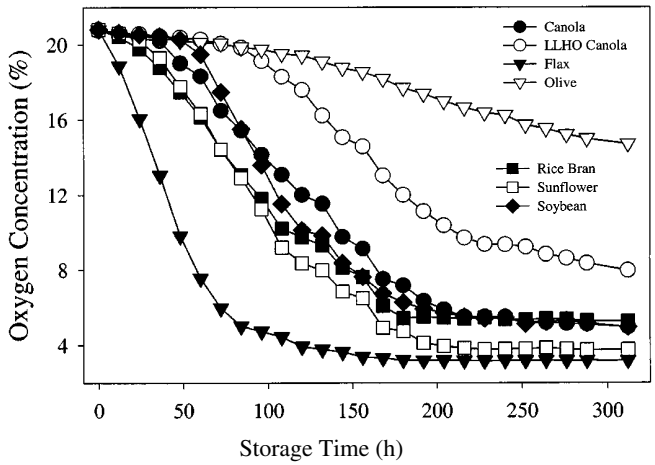

FIG. 2. Oxygen consumption during storage of selected oils at 65°C without light presence. For description see Materials and Methods section. See Figure 1 for abbreviation.

Statistical analysis. Statistical analyses were performed using statistical software package Statistica (Statsoft, Tulsa, OK).

RESULTS AND DISCUSSION

The proper functioning of a Neural Network is highly dependent on the way signals are propagated through the network. During the program training, several settings can be adjusted in order to improve the learning capacity, and consequently improve the predictability of the program. In general, settings are not known beforehand, and the initial choice of parameters is empirical and differs for varying topologies and pattern sets (10,14).

The suitable number of neurons and hidden layers is essential to obtain a well trained program. It is recommended that one hidden layer be the first choice for any practical feedforward network design. More hidden layers may cause overfitting, since the network focuses excessively on the idiosyncrasies of individual samples; however, with too few hidden layers a network may not become trained. The smoothing factor, learning rate, and noise are also reported as important parameters in a training process (5,10,25).

In the present study, better results were obtained when the following parameters were applied: hidden layers 1–2, smoothing factors 0.8–1.0, noise 0–0.05, and learning rates 0.8–1.0. These values were similar to settings published for different applications of ANNW in food quality assessment (6,8,14). It was also observed that the training tolerance, which specifies how close each output of the network must be to the empirical response to be considered correct, markedly affected the training time. As reported by Horimoto *et al.* (14), smaller tolerances required a longer amount of time to train the program. The data sets L_1, L_3, L_4, L_9, D_1, D_2, and D_8 (Table 1) started at a training tolerance of 2.0 and gradually decreased to 1.0. For all other networks, 1.0 was used as the training tolerance.

Predicting stability of vegetable oils during storage with the presence of light. Using a cluster analysis, oils were placed into groups with different oxidative stability, based on k_2 (Fig. 3) Eighteen oils, representing cluster groups, were selected to train the ANNW system, namely, FCO, EPR, CAO, SUR, RBO, SOY, FLL, CTO, CAS, SHO, CAR, ORF, OEV, PLG, COR, PAL, PNT, and COC (Table 1). The other 15 oils were used to test ability of the program to predict the values of k_2.

Several groups of oil components were tested as inputs to verify their ability to predict the stability as measured by k_2 for oxygen consumption measurement. Initially, all individual components measured in the oils, group L_1 (Table 2), were used as inputs, and the values of k_2 were used as outputs. After the program was trained, the remaining 15 oils were used to evaluate the ability of this system to predict this parameter. The r^2 obtained was 0.70 (Table 2). Due to the relatively low predictability, another set of variables was selected to retrain the program, the total amount for each group of components was selected (L_2, Table 1), and a slight improvement in predictability was observed (r^2 = 0.75; Table 2). Horimoto *et al.* (14) found that effective prediction by ANNW can be achieved when the r^2 between predicted and measured values is over 0.90. Therefore, other sets of components (L_3–L_5, Table 2) were individually used to train the program. Based on previous results, the total amount of the components from the particular group was chosen instead of the individual component amounts. For each set of components, the values of k_2 were again predicted by ANNW for the 15 oils tested. As seen on Table 2, a slight improvement in predictability of k_2 was observed, but still the best r^2 of 0.81, was obtained for group L_4.

To improve predictability, the values used to train the program were altered. Two oils, namely PLG and OEV, were re-

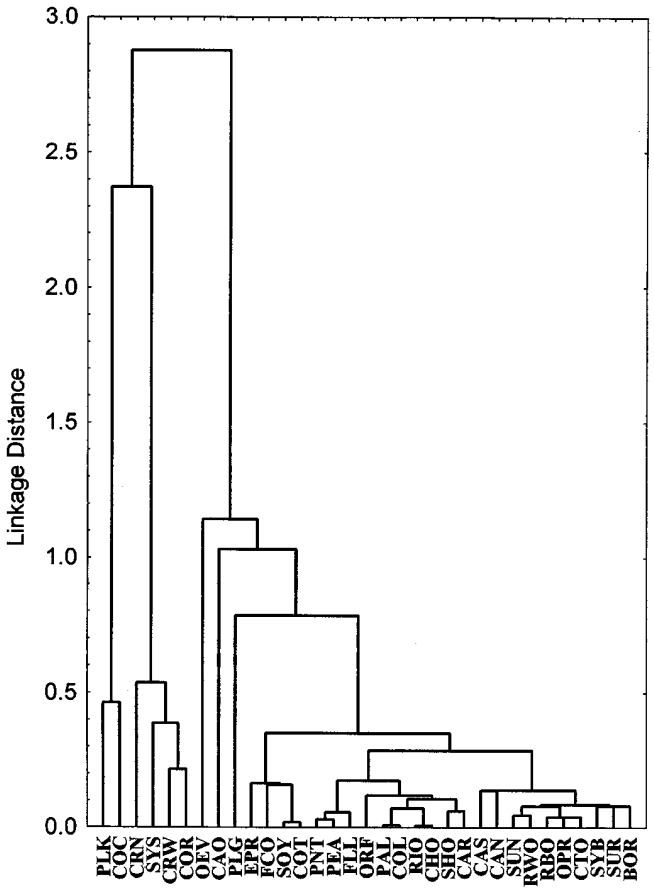

FIG. 3. Cluster analysis of vegetable oils based on slopes of propagation (k_2) as measured during storage at 65°C without light presence. PLK, palm kernel, refined; COC, coconut, pressed and refined; CRN, corn, refined, bleached, and deodorized (RBD); SYS, soybean, RBD; CRW, corn, RBD; COR, corn, RBD; OEV, virgin olive, cold-pressed; CAO, regular canola, RBD, produced from third-grade seeds; PLG, red palm, refined; EPR, evening primrose, cold-pressed; FCO, regular flax, cold-pressed; SOY, soybean, RBD; COT, cottonseed, RBD; PNT, peanut, RBD; PEA, peanut, RBD; FLL, low-linolenic flax, RBD; ORF, olive, RBD; PAL, palm, refined; COL, high-oleic low-linolenic canola, RBD; RIO, rice bran, RBD; CHO, high-oleic canola, RBD; SHO, high-oleic sunflower, RBD; CAR, low-linolenic canola, RBD; CAS, regular canola, RBD; CAN, regular canola, RBD; SUN, regular sunflower, RBD; RBO, rice bran, RBD; RWO, rice bran, RBD and winterized; OPR, olive pomace, RBD; CTO, cottonseed, RBD; SYB, soybean, RBD; SUR, regular sunflower, RBD; BOR, borage, cold-pressed. The same oils with different symbols indicate different processors.

TABLE 1
Groups of Oil Components Used for Training the Artificial Neural Network for Oils Stored with Light Exposure

Groups		Oil components
L_1		Contribution of all individual FA, FFA, NL, PL, GL, tocopherols, tocotrienols, sterols, metals, chlorophyll, carotenoids, and phenolic acids
L_2	D_1	Contribution of linolenic, linoleic, oleic acids; SFA; and the total amount of NL, PL, GL, tocopherols, tocotrienols, sterols, chlorophylls, carotenoids, metals, and phenolic acids
L_3	D_2	Contribution of oleic, linoleic, linolenic acids; SFA; and the total amount of tocopherols and tocotrienols, chlorophyll, metals, sterols, and phospholipids
L_4	D_3	Contribution of oleic, linoleic, linolenic acids; SFA; and the total amount of tocopherols and tocotrienols, metals, sterols, and phospholipids
L_5	D_4	Contribution of oleic, linoleic, linolenic acids; SFA; and the total amount of tocopherols and tocotrienols, chlorophyll, and metals
L_6	D_5	Contribution of oleic, linoleic, linolenic acids; SFA; and the total amount of tocopherols, tocotrienols, chlorophylls, and metals
L_7	D_6	Contribution of oleic, linoleic, linolenic acids; SFA; and the total amount of tocopherols, tocotrienols, chlorophylls, and metals
L_8	D_7	Contribution of oleic, linoleic, linolenic acids; SFA; and the total amount of tocopherols, tocotrienols, and chlorophylls. For training purposes, 22 oils were used
L_9	D_8	Contribution of oleic, linoleic, linolenic acids; and SFA. For training purposes, 22 oils were used.

L_i and D_i, sets of oil components used for training for oils stored with and without light exposure, respectively; FA, fatty acids; FFA, free fatty acids; NL, neutral lipids; PL, phospholipids; GL, glycolipids; SFA, saturated fatty acids contribution.

placed by CHO and OPR in the training set. Both replaced oils were outliers in the total amounts of carotenoids and phenolic compounds, respectively. The program was retrained using this new set of oils with the same variables, contribution of major fatty acids and the amounts of tocopherols, tocotrienols, chlorophylls, and metals (L_6, Table 1) as predictors. By replacing outliers, predictability as measured by r^2 increased to 0.87 (Table 2).

Lawrence and Peterson (25) proposed that using the same number of variables and cases for the training of ANNW can provide better predictability. In the following experiment, the number of oils was equal to the number of groups of components used to train the program. The size of the training oil set was increased to 22, including RWO, SYB, BOR and CRW, oils while the number of components was left the same as in the previous group (L_7, Table 1). A larger r^2 (0.95) was obtained, and the predictability of oxidative stability based on composition was very close to the experimental data generated during oxygen consumption measurements (L_7, Table 2). Among individual oils, OEV had the highest deviation from the experimental data described by standard error of estimation of 18.9×10^{-3}, whereas for the rest of the oils the error was 5.3×10^{-3} (Fig. 4).

Further reduction of the number of oil components used to train and predict oil oxidative stability did not improved predictability (L_8, L_9; Tables 1 and 2). Two new sets of components were tested. Their fatty acid composition with and without the total amount of tocopherols and chlorophylls was used. The last group represents the claim that fatty acids are responsible for oils/fats oxidative deterioration (26). Using fatty acid composition and the amounts of tocopherols and chlorophylls obtained, the r^2 was 0.59, while for fatty acids alone it was 0.44. This indicates that using fatty acid composition as a predictor can only describe half of the oxidative stability of the oil (Table 2).

Predictability of stability for oils stored without light at 65°C. As can be noticed from Figure 2, the induction period for many oils was observed when stored without light presence. This is contrary to the experiments involving storage with light exposure where propagation started from the beginning of the storage time (Fig. 1). This indicates that light and photosensitive components play important roles as oxidation initiators. The model, applied to 22 oils stored with light presence, was applied to train the ANNW system for

TABLE 2
Correlation Coefficients (r^2) and the Standard Errors of Estimation (SEE) for Predicted and Experimental Values of Propagation Slope (k_i) for Selected Group of Oil Components

Group of oil components[a]	r^2	SEE ($\times 10^{-3}$)
L_1	0.7038	4.9
L_2	0.7519	3.3
L_3	0.6827	8.5
L_4	0.8135	6.9
L_5	0.8029	3.0
L_6	0.8746	2.9
L_7	0.9554	3.1
L_8	0.5939	5.6
L_9	0.4458	11.7

[a]For abbreviations, see Table 1.

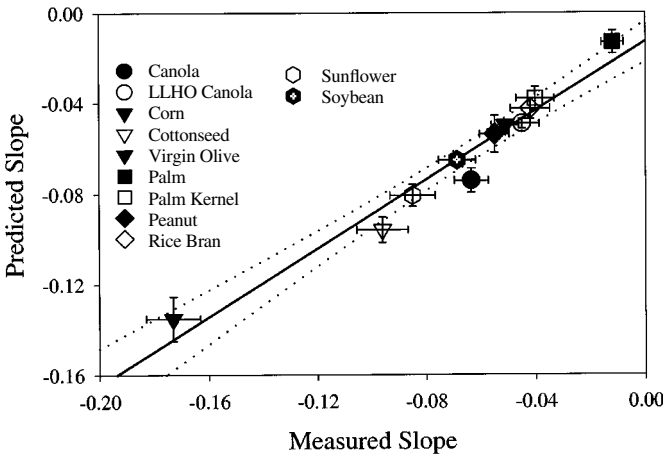

FIG. 4. Correlation between measured and predicted values of slope of propagation (k^2) obtained during storage with light at 35°C. For description see Materials and Methods section. Error bars represent standard error of estimation. See Figure 1 for abbreviation. (—) Regression line (r^2 = 0.955); (·····) 95% confidence levels.

predicting oxidative stability during storage without light presence. Similarly to what was done before, several groups of oil components were selected to test the predictability using ANNW (D_1–D_8, Table 1).

Fatty acid composition and the total amount of components (D_1, Table 2) were used as inputs and the values of k_1, k_2, and the ip were used simultaneously as outputs (three outputs). The correlation coefficients between the values predicted by ANNW and the experimental values from oxygen consumption are presented in Table 3. Values below 0.90 were obtained for r^2 indicating relatively low predictability.

Due to the low r^2 observed for the prediction of k_1, k_2, and ip simultaneously, two new data sets (D_2 and D_3, Table 1) were applied in order to find which oil's endogenous components can better predict stability. As can be noticed from Table 3, even lower r^2 were obtained for these new compositional variables. Even though the ANNW can predict more than one value (one output) at the same time, this program is mostly used to predict a single output (10). For the next attempt, the program was trained to predict each of the mentioned parameters separately, using a set of inputs comprising the major fatty acid composition and total amounts of tocopherols, tocotrienols, chlorophylls, and metals (D_4, Table 3). The r^2 between predicted and experimental values for the ip was markedly improved ($r^2 = 0.91$), but for k_1 and k_2, no improvement was observed (Table 3). Other sets of components were tested (D_5, D_6, D_7, and D_8, Table 1) to find the oil components that could give the best predictability. The best value of $r^2 = 0.95$ was achieved when composition of the major fatty acid with the total amounts of tocopherols, tocotrienols, metals, sterols, and phospholipids was applied (D_5, Table 3). Among individual oils, the highest SEE was found for PLG, 21.1×10^{-3}, while for other oils observed values were below 9.8×10^{-3} (Fig. 5).

Since low predictability was obtained for k_1 and k_2, data from oxygen consumption representing initiation and propagation periods were combined into a single regression. Obtained slopes (k_3) were used as outputs (Table 4) with the following groups of oil components as predictors: D_2, D_3, D_6, D_7, and D_8 (Table 1). Each group of components was run separately with the same output, and after training the system was tested for efficiency in predicting oxidative stability of oils. The best r^2 between predicted and measured values was found when the composition of major fatty acids and the total amounts of tocopherols, tocotrienols, metals, sterols, and phospholipids were used (Table 5, D_2). The r^2 obtained for k_3 as outputs were more satisfactory than for k_1, and k_2 when they were applied individually (Tables 3 and 5).

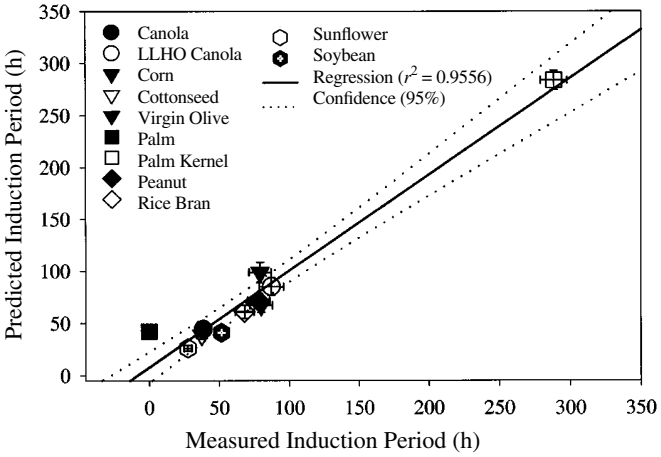

FIG. 5. Correlation between measured and predicted values of initiation period obtained during storage at 65°C. For description see Materials and Methods section. Error bars represent standard error of estimation calculated by Neural Network for predicted data and standard deviation for measured values. See Figure 1 for abbreviations.

The previously discussed set of components that produced the best predictability was used to predict k_3 values for oils and compare them to the values measured by oxygen consumption (Fig. 6). The sets of oil components D_2 and D_5 (Table 2) consisted of the same components, but were used for evaluation of different parameters (Table 1). These oil components gave the highest r^2 of 0.92 and 0.95, respectively (Table 5, D_2; Table 3, D_5). The reduced number of oil components to fatty acids and the total amounts of saturated fatty acids, tocopherol, and to-

TABLE 3
r^2 and the SEE for Predicted and Experimental Values of Parameters Calculated from Oxygen Consumption Measurements During Oil Storage Without Light Exposure

Groups of oil components[a]	r^2			SEE ($\times 10^{-3}$)		SEE
	k_1	k_2	ip	k_1	k_2	ip
D_1	0.7168	0.6542	0.7017	7.5	9.2	6.7
D_2	0.6817	0.5748	0.5448	6.4	7.3	11.3
D_3	0.6357	0.6862	0.6736	5.1	9.7	8.4
D_4	0.6953	0.6381	0.9148	6.1	5.9	1.5
D_5	—	—	0.9521	—	—	3.1
D_6	—	—	0.8875	—	—	2.8
D_7	—	—	0.9139	—	—	1.4
D_8	—	—	0.5362	—	—	14.3

[a]k_1, slope of initiation period; k_2, slope of propagation period; ip, induction period; for other abbreviations, see Table 2.

TABLE 4
Values of k_1 and k_2, ip, and Combined Slope (k_3) Used to Train the Neural Network System

Oils[a]	k_1	k_2	ip(h)	k_3
CAN	–0.0151	–0.0953	38.6	–0.0845
COL	–0.0083	–0.0844	87.1	–0.0541
CRW	–0.0101	–0.1090	79.9	–0.0615
COT	–0.0153	–0.1258	37.5	–0.0910
OEV	–0.0140	–0.0234	79.1	–0.0203
PLG	–0.0000	–0.0540	0.0	–0.0540
PEA	–0.0123	–0.0483	78.1	–0.0370
RIO	–0.0163	–0.0748	68.1	–0.0550
SUN	–0.0240	–0.1160	27.6	–0.1123
SYS	–0.0083	–0.1300	51.5	–0.0990

[a]CAN, regular canola, refined, bleached, and deodorized (RBD); COL, high-oleic low-linolenic canola, RBD; CRW, corn, RBD; COT, cottonseed, RBD; OEV, virgin olive, cold pressed; PLG, red palm, refined; PEA, peanut, RBD; RIO, rice bran, RBD; SUN, regular sunflower, RBD; SYS, soybean, RBD. See Table 3 for other abbreviation.

TABLE 5
r^2 and the SEE for Experimental and Predicted Values of Combined Slope of Oxidation (k_3) When Different Groups of Oil Components Were Used for Prediction with Neural Network System[a]

Factors	D_2	D_3	D_6	D_7	D_8
r^2	0.9238	0.8542	0.8010	0.8876	0.5659
SEE ($\times 10^{-3}$)	1.9	3.3	6.1	4.0	9.2

[a]See Table 1 for abbreviations.

cotrienol (D_7) gave the r^2 of 0.88 for predicted value when compared to the measured value. Using only fatty acids as predictors showed the lowest ability to predict oxidative stability of oils by the ANNW system (Table 5, D_8).

The results from this study suggest that oil stability can be successfully predicted by ANNW using a few oil components as predictors. For both storage conditions, the use of all oil components did not improve predictability of any parameter measured by oxygen consumption in this study. These results suggest that many of the oil components could not be directly involved in the oil oxidative stability, although they can have synergistic or antagonistic effects on other components.

The best predictors for the k_2, as measured by oxygen consumption during storage with light exposure, were the combination of fatty acids composition, and the amounts of chlorophyll, tocopherols, tocotrienols, and metals. This selection verified recent knowledge about the effect of some minor components on oil oxidative stability, where pigments and metals were found to be initiators of the oxidation process (27). Additionally, antioxidants such as tocopherols and tocotrienols were described as important factors affecting oil oxidative deterioration (1). As mentioned previously, composition of fatty acids can only partially explain oil oxidative stability during storage. Composition of fatty acids, the amounts of tocopherols, tocotrienols, sterols, metals, and phospholipids were found to be the best descriptors for the prediction of ip during storage without light exposure. In this case, sterols and phospholipids were found important in describing this behavior of oils. Phospholipids can probably form complexes with metals, and in this way keep them active and/or available as catalysts (27). Sterols, as found before, can also be oxidized. This means that sterols can be treated as possible stimulators of the oxidation and/or intermediates in free radical formation (28).

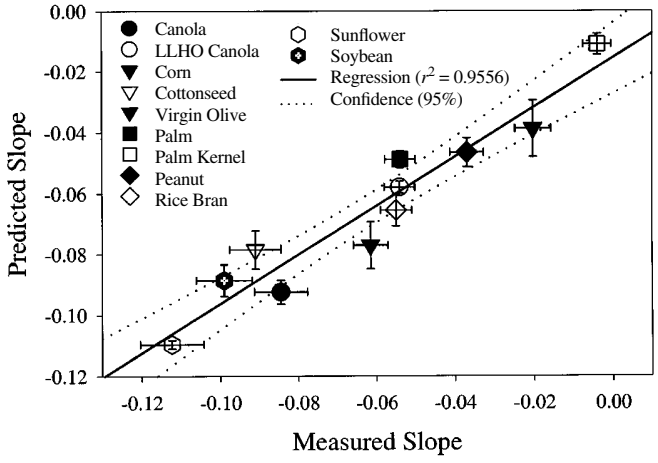

FIG. 6. Correlation between measured and predicted values of combined slope of propagation (k_3) during storage at 65°C without light. For description see methods. Error bars represent standard error of estimation for predicted and measured values. See Figure 1 for abbreviations.

Fatty acid composition with the total amounts of tocopherols and tocotrienols can also be used to predict oxidative stability, as measured by k_2, where r^2 between predicted and experimental values obtained was 0.91. These results suggest that a good predictability of stability of oils stored under both conditions can be obtained by using their fatty acid composition and the total content of tocopherols and tocotrienols. Oxidative stability of vegetable oils can be related to more than unsaturated fatty acids deterioration, and more research is needed to explore the effect of other endogenous components.

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