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Modeling of a Natural Lipstick Formulation using an Artificial Neural Network

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Abstract

An artificial neural network (ANN) was applied in conjunction with experimental data from a mixture of experimental designs to predict the melting point of a lipstick formulation. The experimental data were utilized for training and testing the suggested model. By using the ANN performance results, the optimum parameters were pitaya seed oil 25% w/w, virgin coconut oil 37% w/w, beeswax 17% w/w, candelilla wax 2% w/w, and carnauba wax 2% w/w. The relative

standard error under these parameters is only 0.8772%. It was found that batch back-propagation (BBP) gave the optimal algorithm and topology with a configuration of five inputs, two hidden nodes and one output node; the most important parameter is the carnauba wax content of 24.5%.

Keywords: Color cosmetics, Lipstick, Melting point, Formulation, Artificial neural network, Optimization

Introduction

The cosmetics industry is an enormous worldwide economy worth approximately USD26 billion of which the decorative cosmetics such as lipsticks and makeup accounted for 13% of the market. Decorative cosmetics certainly enhance female attractiveness and impart color to the skin. In modern society, cosmetics are also used to protect the skin from damage by pollutants, ultraviolet light, and personal hygiene.[1] To date, growing attention is being paid to technologically advances in cosmetics products, which has led people to search for cosmetics with natural ingredients and safe resources. Lipstick is one of the decorative cosmetics with high demand in the global market. The practice of lip coloring originated from the ancient prehistoric age. Recently, the use of the lipstick is increasing with the widely available textures, shades of color, and other properties, as well as more advanced technologies.[2] Consumers today are concerned with the importance of their health and not only their outer appearance. They are searching for products from natural sources that are also safe for their health. Lipstick contains variety of waxes, emulsifiers, emollients, preservatives, colorants, and binders in their formulation, which is linked directly to the quality of the lipstick. The solid structure of a lipstick is provided by wax, whereas the moisture in the structure comes from a variety of emollients such as blended oils.[3]

Optimization is one of the effective tools that appear necessary to formulate lipsticks and other cosmetic formulations. In fact, the optimization was carried out by a traditional method, using one variable at a time, which took a lot of time and costs a lot of money. In the traditional method, one of the parameters is varied while the other parameters are kept constant in order to measure the response. So, multivariate methods are the best and widely used to model the input and the effective parameters on the output for optimizing the response. An artificial neural network (ANN) is one multivariate method that models the interaction of the parameters simultaneously during the performance, using universal mathematical learning algorithms including the batch back-propagation (BBP), incremental back-propagation (IBP), genetic algorithm (GA), Levenberg–Marquardt (LM), and quick propagation (QP) algorithms. In a multivariate process, the generated model is used to predict the optimum values of the parameters and their importance.[4-6]

In this work, compositions of blended lipstick ingredients were modeled as effective parameters by the multilayer feed-forward neutral network. The network was trained using QP, IBP, BBP, GA, and LM learning algorithms to obtain the appropriate model. By minimizing the root-mean-squared error (RMSE), the optimum training (topology) of each algorithm was determined. To select the final model for the blended ingredients, the performance of the obtained topology was compared by minimized absolute-average deviation (AAD) and maximized *R*-squared (R^2) tests. The model was used to determine the importance and narrow levels of the effective parameters. Moreover, the appropriate melting point (response) was predicted at the optimum formulation. In fact, this work aims to locate the optimum formulation for natural lipstick through D-optimal mixture experimental design, as an experimental design and ANN, as a statistical tool for optimization.

Experimental Section

Materials

Virgin coconut oil and castor oil were purchased from Euro-Pharma SdnBhd, Pulau Pinang, Malaysia. Pitaya seed was purchased from Great Sun Pitaya Farm, Teluk Panglima Garang, Selangor, Malaysia. *n*-Hexane and ethanol were purchased from Merck, Chemicals, Darmstadt, Germany. Red iron (III) oxide was purchased from Sigma–Aldrich, St. Louis, MO, USA. Beeswax, candelilla wax, and carnauba wax were purchased from Making Cosmetics Inc., Snoqualmie, WA, USA.

Extraction of pitaya seed oil

Pitaya seed oil was extracted using *n*-hexane and ethanol to obtain the unsaturated fatty acids and antioxidants (flavonoid and phenol). A solvent extraction technique was used to obtain the compounds. The pitaya seed (20.0 g) was ground up using a blender and soaked with hexane (450 mL) before being left for overnight for ethanol solvent extraction. The process was repeated three times for each solvent in order to make sure all of the compounds were extracted from the seed.[7]

Formation of Lipstick

A mixture of several oils, natural waxes, and other materials were used as the formulation for this natural-product-based lipstick. The oils were mixed together and homogenized, before the colorant powder was added to ensure the dispersion of the pigment.[8] The blended solution was homogenized using a high-shear homogenizer (IKA T18 Basic ULTRA-TURRAX, Hamburg, Germany) at a speed of 10,000 rpm. The waxes were added to the solution and heated to 85–90°C until they melted. The mixture of blended oils, colorant, and waxes were homogenized

together and other materials were added at the end of the process. All of the blended ingredients were homogenized at a speed of 10,000 rpm for 40 min at 70–80°C to ensure all ingredients are homogenized together. Then, the liquid phase of the lipstick formulation was cooled for 2 hours at –20°C to allow complete crystallization of the waxes in the formulation. The lipstick products were placed in casing and stored overnight before characterization of the melting points.[7]

Artificial Neural Networks (ANNs)

ANNs are generated by direct relationships between the elements recognized as neurons that are able to indicate a link between entrance and exit signals in a specific form, just like the biology of the human brain and body.[9] The input, hidden, and output layers are mathematically free functions of a complicated practical process that are contained within an ANN. The layers consist of several nodes that are connected by a multilayer normal feed-forward or feed-back connection formula.[10]

The hidden layer could be more than one parallel layer, but only a single hidden layer is usually proposed. The user has to define the number of hidden nodes.[11] The nodes of a particular layer are linked to the nodes of the next layer. The nodes are the simple artificial neurons that simulate the behavior of a biological neural network. The nodes of the input layer are authorized by sending data through special weights to the nodes of the hidden layer and then to the output layer.[10] The authorization is achieved by associated weights during the learning process, which is also known as the learning algorithm.

Modeling process

Modeling and optimization of the ingredients was carried out by NeuralPower software version 2.5. [10, 11] To design the experiments, the effective input variables were considered as pitaya seed oil (10–35% w/w), virgin coconut oil (25–45% w/w), beeswax (5–25% w/w), candelilla wax (1–5% w/w), and carnauba wax (1–5% w/w) [7], whereas the melting point was the response of interest, as shown in Table 1. As shown in Table 1, 23 experiments were divided randomly into two data sets, that is, training (15 points) and testing (8 points). The software facilitated randomization. The training and testing data sets were used to compare and ensure robustness of the network parameters, respectively. In addition, the testing set was utilized to avoid over-fitting by controlling the errors.[12]

Table 1 Actual and predicted values of the ANN based on BBP model of lipstick formulation.

Run No.	A	B	C	D	E	Melting point (^{o}C)	
	(%w/w)	(%w/w)	(%w/w)	(%w/w)	(%w/w)	Actual	Predicted
Training Set							
1	35.00	33.21	8.49	4.99	1.29	41.00	40.93
2	35.00	33.21	8.49	4.99	1.29	41.00	40.93
3	10.19	39.74	25.00	4.99	3.09	49.00	50.06
4	22.99	44.85	5.166	5.00	4.99	44.00	44.27
5	24.43	29.36	21.11	5.00	3.10	50.00	49.12
6	14.99	45.00	16.90	1.07	4.99	48.00	48.27
7	10.91	44.98	25.00	1.11	1.00	51.00	48.53
8	26.41	25.60	25.00	1.00	4.99	49.00	49.09
9	34.99	33.15	8.29	1.58	5.00	43.00	41.96
10	34.97	25.00	13.85	4.99	4.19	49.00	47.80
11	17.76	44.99	15.38	3.86	1.00	46.00	46.23
12	28.73	25.20	24.99	3.08	1.00	45.00	46.53
13	26.87	34.36	18.68	1.00	2.09	45.00	45.27
14	34.99	33.15	8.29	1.58	5.00	41.00	41.96
15	10.91	44.98	25.00	1.11	1.00	48.00	48.53
Test Set							
1	28.73	25.20	24.99	3.08	1.00	47.00	46.53
2	28.55	31.96	12.51	4.99	4.99	49.00	48.62
3	10.08	40.85	25.00	2.65	4.42	50.00	50.06
4	26.41	25.60	25.00	1.00	4.99	49.00	49.09
5	10.07	45.00	17.96	4.98	4.97	50.50	49.95
6	28.98	45.00	6.35	1.27	1.41	37.00	37.80
7	19.07	37.65	19.84	1.98	4.47	51.00	49.19
8	12.76	35.33	24.92	4.99	5.00	49.00	50.22

A: Pitaya seed oil; B: Virgin coconut oil; C: Beeswax; D: Candelilla wax; E: Carnauba wax

The Learning Process

The weights are calculated by the weight of summation [Eq. (6)] of the received data from the former layer and transfer layer in the learning process.[13] The number of hidden nodes is obtained by trial-and-error training calculations, which are examined between one and *n* nodes. The output of the hidden nodes, in turn, acts as the input/output layer nodes, which undergo similar or different transformations.

The common learning algorithms are BBP, IBP, QP, LM, and GA, whereas multilayers are the connection-type nodes.[14] The logarithmic sigmoid represents the usual transfer function for both hidden and output layers that are bounded from 0 to 1.[15] The input and output data that are provided by the software scaling are normalized by the sigmoid. The scaled data are passed into the first layer, propagated to the hidden layer, and then finally meet the output layer of the network. Each node in an output or hidden layer acts as a summing junction, which modifies the inputs from the previous layer, using the following equation:

$$y_i = \sum_{j=1}^{i} x_i w_{ij} + b_j \qquad (1)$$

where y_i is the input of the network to the *j* node in the hidden layer, i is the number of nodes, x_i is the output of previous layer, and w_{ij} is the weight of the connection between the ith and *j*th nodes. The bias associates with node *j* that is presented by b_j. The main objective of the

process is to find the weights required to minimize the RMSE, which is obtained from the difference between network prediction and the actual responses.

$$\mathrm{RMSE} = (\frac{1}{n}\sum_{i=1}^{n}(y_i - y_{di})^2)^{\frac{1}{2}} \qquad (2)$$

where n the number of the points, y_i is the predicted value, and y_{di} is the actual value. Therefore, the learning process with an algorithm is continued until the minimum RMSE is found, which is called the topology. The learning of the topology is repeated several times to avoid random initialization of the weight. As a result, the topology with the lowest RMSE is selected and compared with the topologies of other nodes. Therefore, the topologies for *n* hidden layers of the considered algorithms are obtained in same way. Finally, the topologies of the algorithms are compared in order to select a provisional model with the maximum R^2 [Eq. (3)] and minimum RMSE and AAD values [Eq. (4)].

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - y_{di})^2}{\sum_{i=1}^{n}(y_{di} - y_m)^2} \qquad (3)$$

$$\mathrm{ADD} = \frac{1}{n}\sum_{i=1}^{n}\frac{|\, y_i - y_{di}\,|}{y_{di}} \times 100 \qquad (4)$$

where n represents the number of points, y_i is the predicted value, y_{di} is the actual value and y_m is the average of the actual values.

Batch Back-Propagation (BBP) Algorithm

BBP is one of the back-propagation algorithms that operates batch-mode training and provides an accurate estimation of a gradient vector and convergence to a local minimum under simple conditions.[9, 16] The gradient algorithm is bound and naturally convergent.[17] Owing to the high nonlinearity of the neural network, this optimal step size was difficult to find when we applied a gradient method. Therefore, the learning rate for BBP is usually set to achieve an adaptive or constant series.[18]

Result and Discussion

Modeling Process

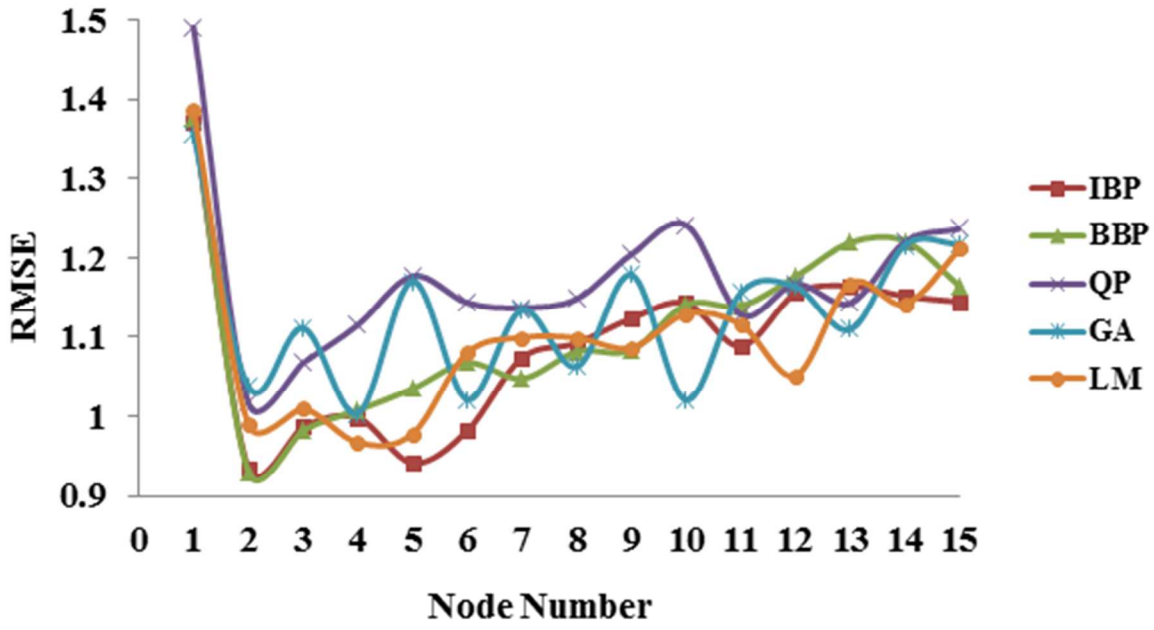
Topologies of the algorithms

An experimental data set with different amounts of ingredients was used for the training and testing of the neural network model. The network of blended ingredients was organized into five nodes as input layers, that is, pitaya seed oil, virgin coconut oil, beeswax, candelilla wax, and carnauba wax, whereas the melting point of the lipstick was the only node in the output layer. A series of topologies with varied node number (from 1 to 15) for each algorithm was examined to determine the structure of the hidden layers.

The model learning was performed for the testing data set to determine the minimum value of the RMSE function. The performance was repeated ten times for each node to avoid random correlation through the random initialization of the weight.[19] The training was carried out in an identical manner for the IBP, BBP, QP, GA, and LM algorithms to find the optimized topology for each one. The minimum value of the RMSE was selected and plotted versus the nodes of the

algorithms' hidden among ten times the learning repetition data for each node (Fig. 1). As shown, one node of 15 topologies for each algorithm presented the lowest RMSE, which was selected as the best topology for comparison purposes. The selected topologies were IBP-5-2-1, BBP-5-2-1, QP-5-2-1, GA-5-4-1, and LM-5-4-1. As shown in Figure 1, the topology of BBP-5-2-1 presented the lowest RMSE among the topologies, so it was selected as a provisional model for the blended ingredients.

Fig 1 **S**elected RMSE vs. node number of the lipstick formulation network hidden layer for IBP, BBP, QP, GA and LM. The lowest RMSE belong to node 2 (IBP), 2 (BBP), 2 (QP), 4 (GA), 4 (LM).

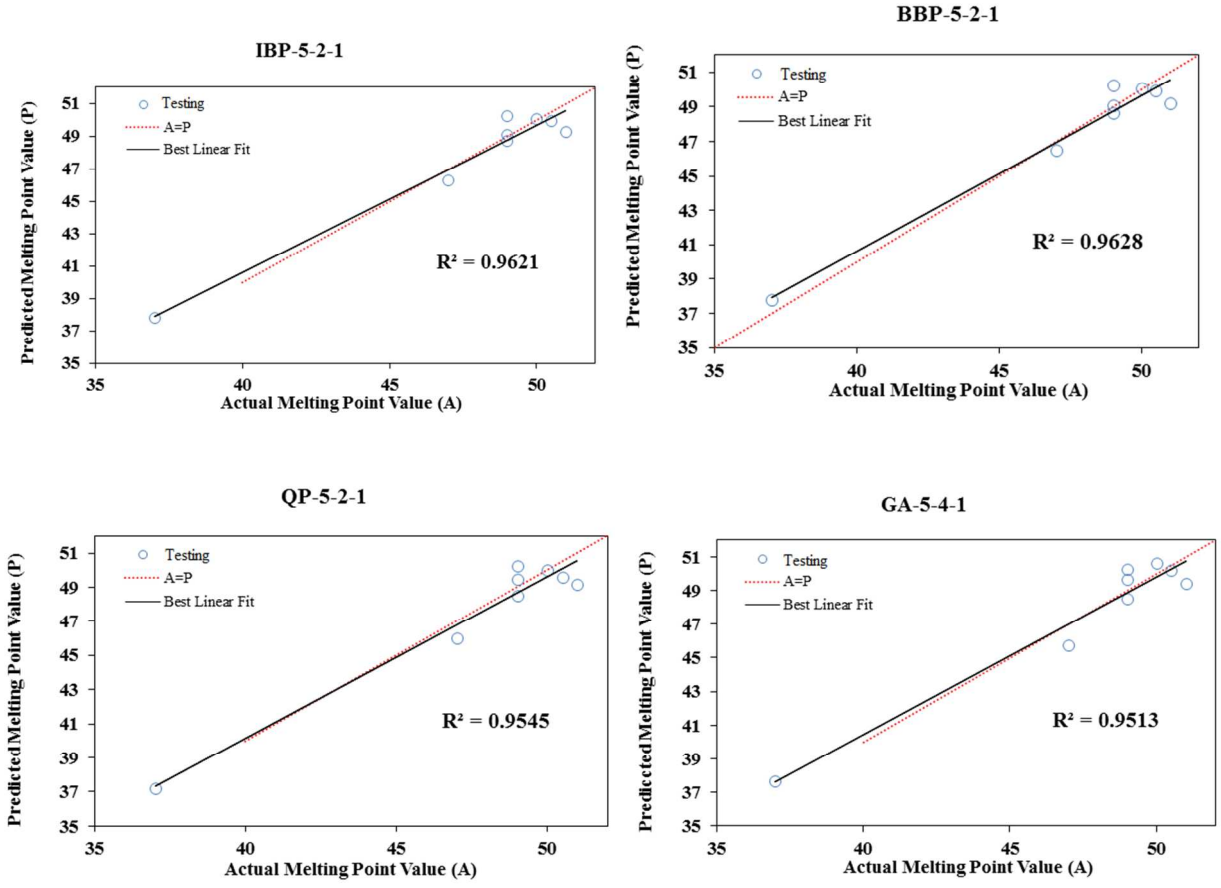


Model selection

For the selection of final model for the blended ingredients, the values of the RMSE, R^2, and ADD were investigated, relatively, for the topologies of IBP-5-2-1, BBP-5-2-1, QP-5-2-1, GA-5-4-1, and LM-5-4-1. To calculate the R^2, the topology predictions and the actual values of the

melting points were plotted for the testing data set (Fig. 2); the R^2 for training set was carried out in a similar way (Fig. 3). As shown in the scatter plots, BBP-5-2-1 presented the highest R^2 for testing (0.96280) and training (0.91430) data sets. However, the AAD of the topologies for the testing and training sets was calculated according to Table 2. As can be seen, the lowest value belongs to BBP-5-2-1. As a result, BBP-5-2-1 was a pioneer with minimum RMSE and ADD values as well as the maximum R^2 among the topologies for the testing and training data sets. So, BBP-5-2-1 was finally selected as the optimum model for the blended ingredients.

Fig 2 Scatter plot of predicted melting point (^{O}C) value *versus* actual melting point (^{O}C), using five algorithms for testing set



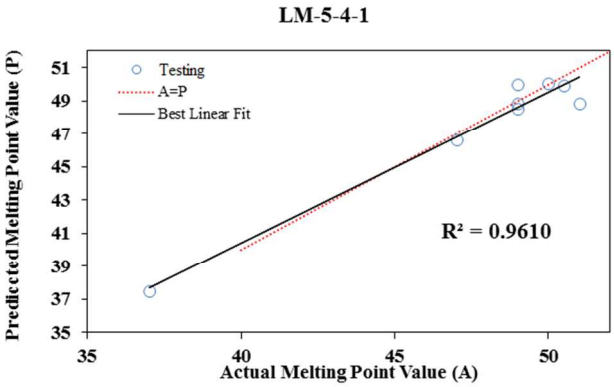
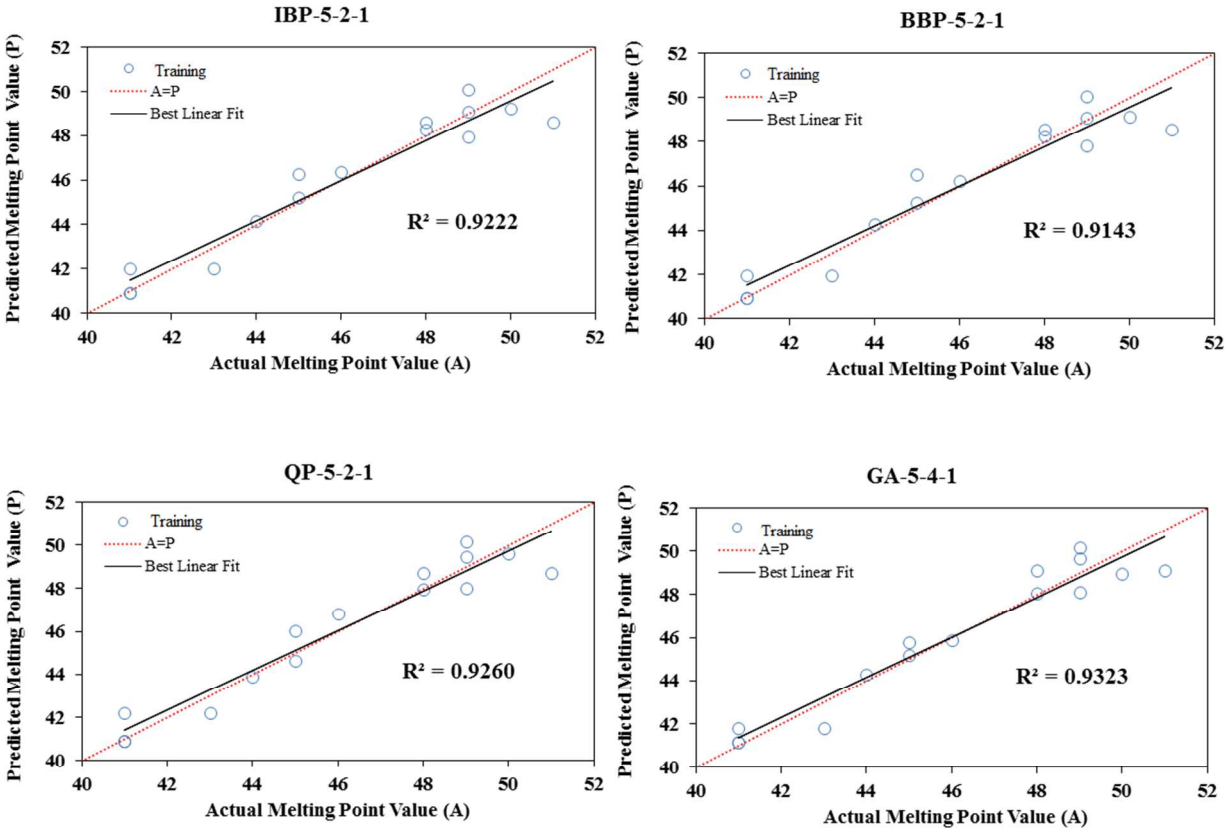


Fig 3 Scatter plot of predicted melting point (^{O}C) value *versus* actual conversion (^{O}C), using five algorithms for training data set.



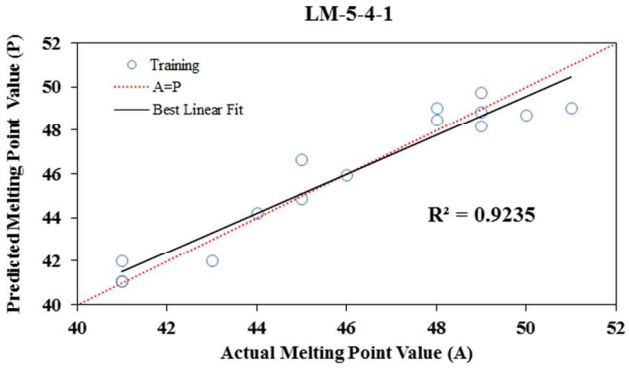


Table 2 The performance results of the optimized topologies of the lipstick formulation: GA-5-4-1, BBP-5-2-1, LM-5-4-1, QP-5-2-1, and IBP-5-2-1.

Learning algorithm	Architecture	Training data			Testing data		
		RMSE	R^2	AAD	RMSE	R^2	AAD
GA	5-4-1	0.8657	0.9323	1.4784	1.0035	0.9513	1.7643
BBP	5-2-1	0.9769	0.9143	1.5519	0.9302	0.9628	1.4196
LM	5-4-1	0.9251	0.9235	1.5132	0.9670	0.9610	1.4363
QP	5-2-1	0.9054	0.9260	1.5087	0.9545	0.9545	1.5711
IBP	5-2-1	0.9306	0.9222	1.4779	0.9345	0.9621	1.4508

Model validation

The BBP-5-2-1 network

The BBP-5-2-1 network was used as the final model for the blended ingredients, which consists of input, hidden, and output layers, as shown in Fig. 4. The input layer with five nodes (pitaya seed oil, virgin coconut oil, beeswax, candelilla wax, and carnauba wax) is the distributor for the hidden layer with five nodes, which were determined through the learning process. The input data of the hidden nodes were calculated by a weighted summation [Eq. (6)].[20] Then, using a log-

sigmoid function [Eq. (7)], the output data of the hidden layer are transferred to the output layer, that is, the melting point.[21]

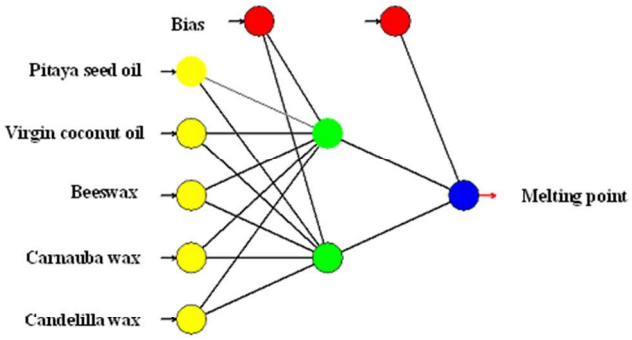
$$S = \sum_{i=1}^{nh} (b - W_i I_i) \qquad (6)$$

where S is the summation, b is the bias, I_i is the ith input to the hidden neuron, and W_i is the weight associated with I_i. The bias shifts the space of the nonlinearity properties.

$$f(x) = \frac{1}{1 + \exp(-x)} \qquad (7)$$

where $f(x)$ is the hidden output neuron. As the result, BBP-5-2-1 was used to determine the importance and the optimum values of the input variables of the blended ingredients in lipstick to achieve the desirable melting point.

Fig 4 Schematic representation of a multilayer perceptron feed-forward network of ANN based on BBP, consisting of five inputs, one hidden layer with two nodes and one output.



The navigation of blended ingredients

In the modeling process, the optimized topologies for different learning algorithms were confirmed by training and testing the data set. The comparison was performed to explain the best relative topology with optimum R^2, RMSE, and ADD values, which was chosen as the provisional model for further evaluation. The adequacy of the chosen model (BBP-5-2-1) was determined by testing the data set. As a result of the process, the BBP-5-2-1 network was chosen to navigate the blended ingredients. The navigation contained a graphical optimization of the effective variables and identified the importance of them. The predicted optimum importance of pitaya seed oil, virgin coconut oil, beeswax, candelilla wax, and carnauba wax, which were used experimentally to obtain the actual melting point (46℃), are shown in Table 3. The actual melting point, within reasonable error, was quite close to the value of the model prediction.

Table 3 Optimum conditions derived by an ANN based on BBP model for lipstick formulation.

Method	Independent Variables					Melting point (^{o}C)		
	A (% w/w)	B (% w/w)	C (% w/w)	D (% w/w)	E (% w/w)	Actual Value	Predicted Value	RSE (%)
ANN-BBP	25.00	37.00	17.00	2.00	2.00	46.00	45.6	0.8772

A: Pitaya seed oil; B: Virgin coconut oil; C: Beeswax; D: Candelilla wax; E: Carnauba wax

Comparison of the ANN Model and D-optimal Mixture Experimental Design (MED)

The two methods were assessed under optimum conditions and the obtained melting points were compared. The effects of the five independent variables (pitaya seed oil, virgin coconut oil. beeswax, candelilla wax, and carnauba wax) are shown in Table 4, along with the predicted values for the melting point of the lipstick. The experiment was performed under the

recommended conditions and the resulting response was compared to the predicted values.[11] The resulting melting point of the lipstick was 46℃. The ANN gave the melting point value as 45.6℃, and these two values are similar. For the D-optimal MED, the melting point value was 45.5℃. Therefore, the ANN model predicted well compared to D-optimal MED, because the ANN model had a lower RMSE compared to D-optimal MED.

Table 4 Optimum conditions derived by an ANN based on BBP and D-optimal mixture experimental design (MED) model for lipstick formulation

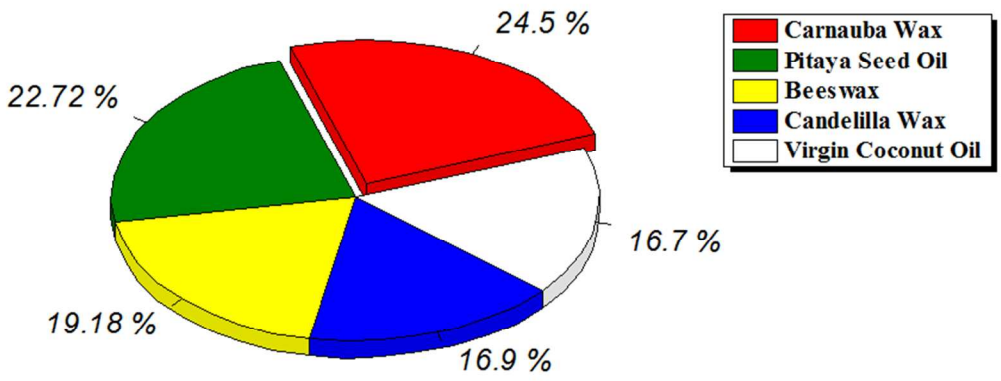
Method	Independent Variables					Melting point (°C)		
	A (% w/w)	B (% w/w)	C (% w/w)	D (w/w %)	E (% w/w)	Actual Value	Predicted Value	RSE (%)
ANN-BBP	25	37	17	2	2.00	46	45.6	0.8772
MED	25	37	17	2	2.00	46	45.5	1.0990

A: Pitaya seed oil; B: Virgin coconut oil; C: Beeswax; D: Candelilla wax; E: Carnauba wax

Importance of the Effective Variables

The models determined the relative importance of the blended effective variables at the optimum melting point (Fig. 5). As the observed, carnauba wax, with a relative importance of 24.5%, appeared to be the most influential on the melting point. Nevertheless, the effects of others variables such as pitaya seed oil, beeswax, candelilla wax, and virgin coconut oil also strongly impacted on the melting point. As a result, none of the variables could be abandoned in this work.

Fig 5 The relative importance of the input variables in lipstick formulation, consisting of pitaya seed oil, virgin coconut oil, beeswax, carnauba wax and candelilla wax.



Conclusion

The effect of various ingredients such as pitaya seed oil, virgin coconut oil, beeswax, candelilla wax, and carnauba wax was investigated in terms of the melting point of lipstick through an ANN method. To obtain the certified network, dissimilar algorithms such as QP, IBP, BBP, GM, and LM were learned by using training and test data sets. The results of the learning program gave five topologies: IBP-5-2-1, BBP-5-2-1, QP-5-2-1, GA-5-4-1, and LM-5-4-1. The topologies were assessed by optimization through RMSE, ADD, and R^2 values. The BBP-5-2-1 topology was chosen as a provisional network of the blended ingredients for the test set, because it had the lowest RMSE and ADD as well as the highest R^2. The result of test data set certified its good ability to predict the model. The testing set model determined the optimum values and relative importance of the effective variables. The importance of the variables included carnauba wax (24.4%), pitaya seed oil (22.72%), beeswax (19.18%), candelilla wax (16.9%), and virgin coconut oil (16.7%), which shows that none of the variables could be neglected in this work. The

results confirmed that neural network modeling could effectively reproduce the experimental data for the formation of lipstick and other cosmetics in the industry.

Conflict of Interest statement

The authors declare no conflict of interest regarding the publication of this work.

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