Modeling of Natural - lipstick formulation by artificial neural network

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Abstract

An artificial neural network (ANN) was applied in conjunction with experimental data from mixture experimental design to predict the melting point of lipstick formulation. The experimental data were utilized for training and testing of the suggested model. By using performance of ANN, 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) as the optimal algorithm and topology with configuration of 5 inputs, 2 hidden and 1 output nodes; respectively with the most importance relative parameter is carnauba wax 24.5%.

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

1. Introduction

The cosmetics industry is an enormous worldwide economy worth approximate about USD26 billion (Barton, 2008) which are the decorative cosmetics such as lipsticks and make-up filled up 13% of the market. Decorative cosmetics certainly enhance female attractiveness and impart the color to the skin. In modern society, cosmetics also used for protect the skin from damaging by pollutant ultraviolet light, personal hygiene and personal hygiene. (Hashim et al., 2009). To date, a growing up attention to technologically advance cosmetics products led people to search cosmetics with compliance natural ingredients and safe resources. Lipstick is one of the decorative cosmetics that demand in global market as one of the successful industry. Lip coloring practice is originated from the ancient prehistoric age. Recently, the use of the lipstick is increasing widely with the available texture, shades of color and others' properties of today's lipstick as well as more advance technologies (Bono et al., 2007). Consumers todays' are concerned of the importance of their health not only their outer appearance. They are searching the products with natural-based and safe for their health. Lipstick contains variety of waxes, emulsifiers, emollients, preservatives, colorants and binders which are the basic materials used in the formulation is linked directly to the quality of the lipstick. Solid structure of lipstick is provided by wax while moisture structure came from varieties of emollients such as blended of oils (Kruthika et al., 2014).

Optimization is one of the effective tools appears necessary to formulate the lipsticks and other cosmetics formulation. In facts, the optimization was carried out by the traditional method such as one variable at a time method was took a lot of time and costs. In the method, one of the parameter is varying while the others parameters are kept constant to measure the response. So, multivariate methods are the best and widely used to model the input, effective parameters to the output for optimizing the response. An artificial neural network is one of the multivariate methods that model the interaction of the parameters simultaneously during the performance by using universal mathematical learning algorithms. The algorithms are batch back-propagation (BBP), incremental back-propagation (IBP), genetic algorithm (GA), Levenberg-Marquardt (LM) and quick propagation (QP). In the multivariate process, the generated model is used to predict the optimum values of parameters and its importance.

In this work, the compositions of blended ingredients of lipstick were modeled as effective's parameters by the multilayer feed-forward neutral network. The network was trained by using QP, IBP, BBP, GA and LM learning algorithms in order to obtain the appropriate model. By minimizing the root mean squared error (RMSE), the optimum trainings (topology) of each algorithm were determined. To select the final model of the blended ingredients, the performance of obtained topologies was compared by minimized absolute average deviation (AAD) and maximized R-squared (R^2). 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 works aim to locate the optimum formulation for natural-lipstick through D-optimal Mixture Experimental Design as an experimental design and artificial neural network (ANN) as a statistical tool for optimization.

2. Experiment

2.1 Material

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.

2.2 Methods

The modeling and optimizing of the ingredients was carried out by NeuralPower software version 2.5 (Abdullahi et al., 2013, Ghaffari et al., 2006, Masoumi et al., 2013). To design the experiments, the levels of the effective input variables considered such as pitaya seed oil (10-35%), virgin coconut oil (25-45%), beeswax (5-25%), candellila wax (1-5%) and carnauba wax (1-5%) (Kamairudin et al., 2014) while the melting point was the interested response as shown in Table 1.

Pitaya seed oil was extracted using *n*-hexane and ethanol to extract the unsaturated fatty acids and antioxidant (flavonoid and phenol). Solvent extraction technique was used to extract the compounds. 20.0g of pitaya seed was grounded using a blender and soaked with hexane (450ml) and left for overnight as well as for ethanol solvent extraction. The process was repeated three times for each solvent in order to make sure all the compounds were extracted from the seed.

A blended of several oils, natural waxes and other materials were used as formulation for this natural based lipstick. The oils are mixed together and homogenized followed by adding the colorant powder to ensure the dispersion of the pigment (Bryce 1993). The blended solution was homogenized by using high shear homogenizer (IKA T18 Basic ULTRA-TURRAX, Hamburg, Germany) at speed 10,000 rpm. The waxes were added into the solution and heated to 85-90 ℃ until they melted. The mixture of blended oils, colorant and waxes were homogenized together and other materials were added at the end. All the blended ingredients were homogenized at speed 10.000 rpm for 40 minutes at 70-80 ℃ to make sure all the ingredients are homogenized together. Then, the liquid phase of lipstick formulation was cooled for 2 hours at -20 ℃ to allow the complete crystallization of the waxes present in the formulation.

The stick lipstick products were placed in casing and stored overnight before characterization for melting point. As shown in Table 1, 23 experiments were divided randomly into two data sets such as training (15 points) and test (8 points). The software facilitated the option of the randomization. The training and testing data sets were used to compare and make sure robustness of the network parameters, respectively. Besides, the testing set was utilized to avoid over fitting by controlling errors (Moghaddam et al., 2010).

2.3 Artificial Neural Networks (ANNs)

Artificial Neural Networks are generated by the straight relationships between the elements recognized as neurons which are able to indicate the link between entrance and exit signal in specific form, just like the biology of human brain and body (Haykin, 2008). The input, hidden and output layer are mathematical free functionalization of the complicated practical process that contain in artificial neural network. The layers consists of several nodes are connected by multilayer normal feed-forward or feed-back connection formula (Ghaffari et al., 2006).

The hidden layer could be more than one parallel layer but the single hidden layer is probably proposed. User had to define the number of hidden layer nodes (Masoumi et al., 2011). The nodes of the particular layer are linked to the nodes of the next layer. The nodes are the simple artificial neurons which simulate the behavior of biological neural network. The nodes of input layer are authorize by sending data through special weights to the nodes of hidden layer and then to the output layer. (Ghaffari et al., 2006, Garson, 1991). The authorization is done by associated weights during learning process also known as learning algorithm.

2.4 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 (Khare and Nagendra, 2007). The number of hidden nodes is gained by trial and error training calculation which is examined from one to *n* nodes. The output of the hidden nodes in turn, acts as input output layers' nodes which undergoes similar or different transformation.

The common learning algorithms are BBP, IBP, QP, LM and GA while the multilayer is the nodes connection type (Salari et al., 2005). The logarithmic sigmoid is the usual transfer function for both hidden and output layers that is bounded from (0-1) (Abdullahi et al., 2013). The input and output data that are provided by the software scaling is normalizing by the sigmoid bounded. The scaled data are passed into the first layer, propagated to hidden layer and finally meet the output layer of the network. Each node in output or hidden layers 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 *j* node in hidden layer i is the number of nodes, x_i are the output of previous layer while w_{ij} are the weights of connection between the ith node and *j*th node. The bias associates with node *j* that is presented by b_j. The main objective of the process is to find the weights for minimizing the error of RMSE which is obtained from difference between network prediction and 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 values and y_{di} is the actual values. Therefore, the learning process with an algorithm is continued until finding the minimum RMSE which is called topology. The learning of topology is repeated several times to avoid random initialization of the weights. As a result, the topology with the lowest RMSE is selected to compare with other nodes' topologies. Therefore, topologies for the *n* numbers of hidden layer for the considered algorithms are obtained in same way. Finally, the topologies of the algorithms are compared to select the provisional model by maximum R^2 (Eq. (3)) and minimum RMSE and AAD (Eq. (4)).

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

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

where n is 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 algorithm

Batch back propagation (BBP) is one of the back propagation algorithm which is batch mode of training provides an accurate estimation of gradient vector, convergence to a local minimum is there by guaranteed under simple condition (Rumelhart and McClelland, 1986, Haykin, 1994 and Heskes and Wiegerinck, 1996). The gradient algorithm is bounded and convergent naturally (Zhang et al., 2012). Because of the high nonlinearity of neural network, this optimal step size was difficult to find when we applied gradient method. Therefore, the learning rate for BBP is usually set to be given adaptive or constant series (Didandeh et al., 2011).

3. Result and discussion

3.1 Modeling process

3.1.1 The topologies of the algorithms

Experimental data set at different amount of ingredients was used for training and test set of neural network model. The network of the blended ingredients has been organized of five nodes such as pitaya seed oil, virgin coconut oil, beeswax, candelilla wax, and carnauba wax, in input layer while the melting point of the lipstick was only the node in 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 testing data set to determine the minimum value of RMSE as error function. The performance was 10 times repeated for each node to avoid random correlation due to the random initialization of the weight (Kasiri et al., 2008). The training was identically carried out for IBP, BBP,QP, GA and LM algorithms to find the optimized topology for each algorithm. The minimum value of RMSE was selected and plotted *vs.* the nodes of the algorithms' hidden among 10 times the learning repetition data for each node (Fig. 1). As shows, one node of 15 topologies for each algorithm has presented the lowest RMSE which was selected as the best topology for comparison. The selected topologies were IBP-5-2-1, BBP-5-2-1, QP-5-2-1, GA-5-4-1 and LM-5-2-1. As shown in Fig. 1, the topology of BBP-5-2-1 presented the lowest RMSE among other topologies that was selected as provisional model for the blended ingredients.

The model selection

For the selection of final model of the blended ingredients, the values of RMSE, $R^2$and ADD were relatively investigated for the topologies of IBP-5-2-1, BBP-5-2-1, QP-5-2-1, GA-5-4-1 and LM-5-2-1. To calculate the R^2, the topologies prediction and actual values of the melting points were plotted for testing data set (Fig. 2) as well as the R^2 for training set was carried out in similar way (Fig. 3). As shown in scatter plots, BBP-5-2-1 has presented the highest R^2 for testing (0.9628) and training (0.9143) data sets. However, the AAD of testing set and training sets for topologies was calculated by Table 2. As seen, the lowest value belongs to BBP-5-2-1. As a result, BBP-5-2-1 was pioneer in minimum RMSE and ADD as well as at maximum R^2 among the topologies for testing and training data sets. So, BBP-5-2-1 was selected as final optimum model of the blended ingredients.

Model validation

The network of BBP-5-4-1

The network of BBP-5-2-1 as a final model for the blended ingredients which consists of inputs, hidden and outputs layers as shown in Fig.4. The input layer with 5 nodes (pitaya seed oil, virgin coconut oil, beeswax, candelilla wax and carnauba wax) is the distributor for the hidden layer with 5 nodes which were determined by learning process. The input data of hidden nodes are calculated by weighted summation (Eq. (6)) (Zhang et al., 1998). Then, by using log-sigmoid function (Eq. (7)) the output data hidden layer are transferred to output layer (melting point) (Aijun et al., 2004).

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

where S is summation, b is bias, I_i is the ith input to 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.

The navigation of blended ingredients

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

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

The two methods were assessed under optimum conditions point for melting point was 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 lipstick. The experiment was done under recommended conditions and resulting response was compared to the predicted values (Masoumi et al., 2013). The resulting melting point of the lipstick is 46℃. The ANN gave the melting point value is 45.6 ℃ which is quite close to the predicted. For D-Optimal Mixture Experimental Design (MED), the melting point value was 45.5℃. Therefore, ANN Model predicted well compared to D-optimal Mixture Experimental Design (MED) because ANN Model has lower value of RSE compared to D-optimal Mixture Experimental Design.

3.2 Importance of the effective variables

The model has been determined the relative importance of the blended effective variables at optimum melting point (Fig. 5). As the observed, carnauba wax with the 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 were strongly on the melting point. As a result, none of the variables is abandon in this work.

4. Conclusion

The effect of various ingredients such as pitaya seed oil, virgin coconut oil, beeswax, candelilla wax and carnauba wax were investigated for the melting point of lipstick through artificial neural network method. To obtain the certified network, the dissimilar algorithms such as QP, IBP, BBP, GM and LM were learned by using training and test data sets. The results of learning program were 5 topologies likes IBP-5-2-1, BBP-5-2-1, QP-5-2-1, GA-5-4-1 and LM-5-2-1. Topologies were performed by optimizing through RMSE, ADD and R^2. The topology (BBP-5-2-1) was chosen as provisional network of the blended ingredients for test set because had the lowest RMSE, ADD and highest R^2. The result of test data set certified the high ability to predict the model. The testing set model has determined the optimum values and relative importance of the effective variables. The importance of the variables was 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 none of the variables is neglect able in this work. The results confirmed that the neural network modeling could effectively reproduce the experimental data for the formation of lipstick and other cosmetic industry.

Conflict of Interest statement

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

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Fig. 1. The selected RMSE vs. node number of the lipstick formulation network's 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).

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

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

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.

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

Table list:

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

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

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

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

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Fig 1:

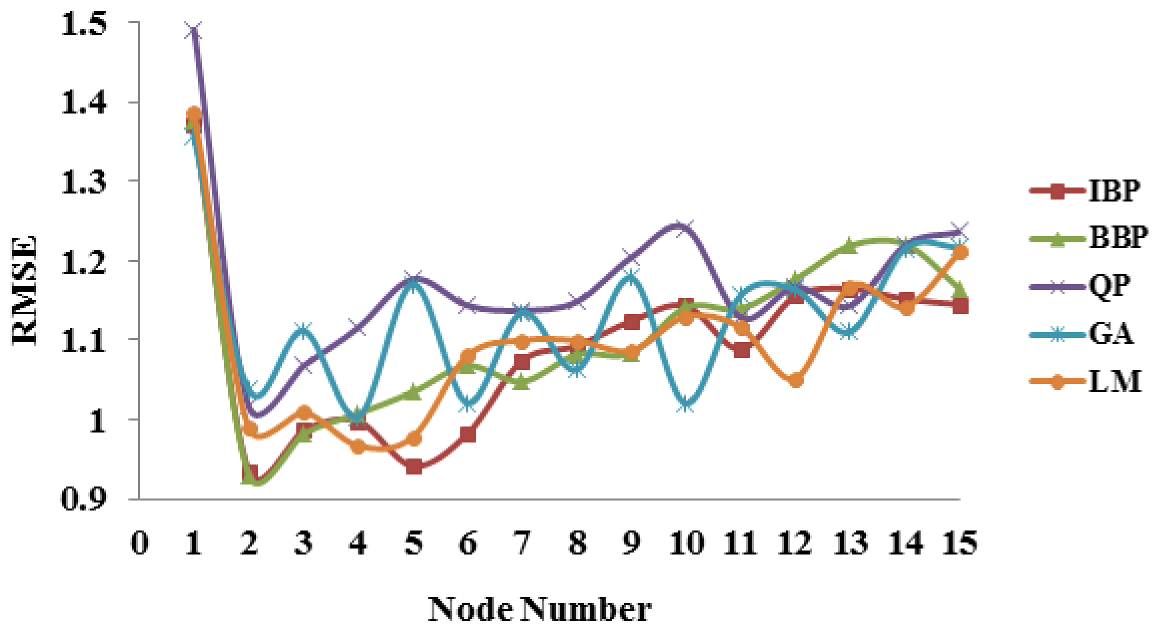
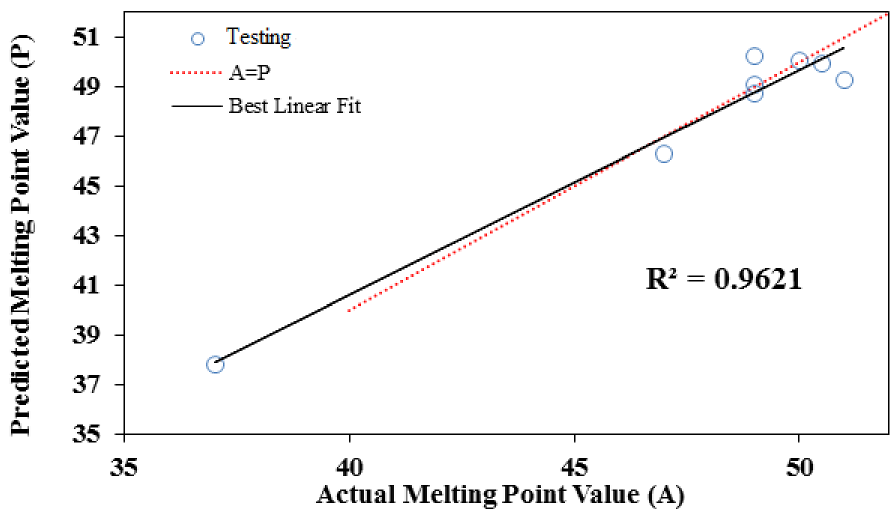

1.5
1.4
1.3
1.2
1.1
1
0.9
RMSE
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
Node Number
IBP
BBP
QP
GA
LM

Fig 2:

IBP-5-2-1



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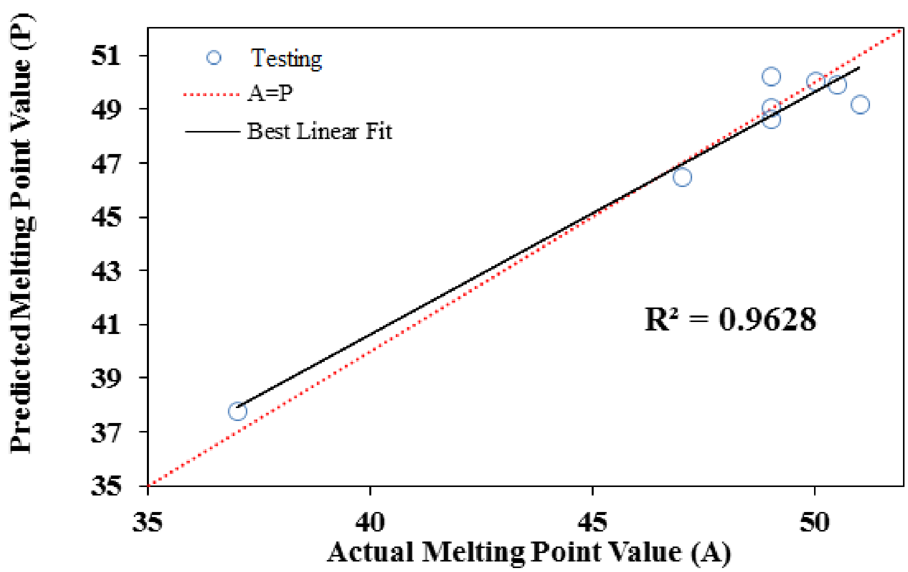

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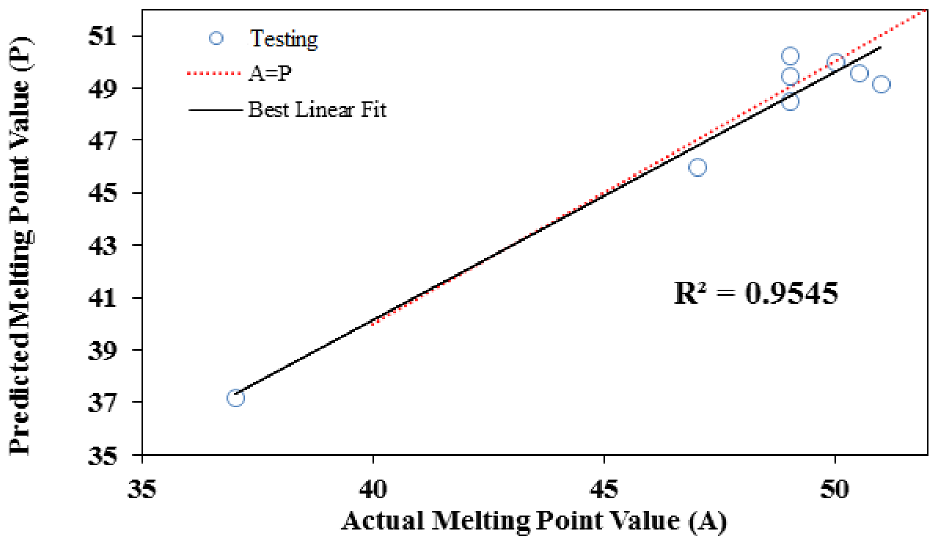
Testing
A=P
Best Linear Fit
R² = 0.9545
Predicted Melting Point Value (P)
Actual Melting Point Value (A)
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49
47
45
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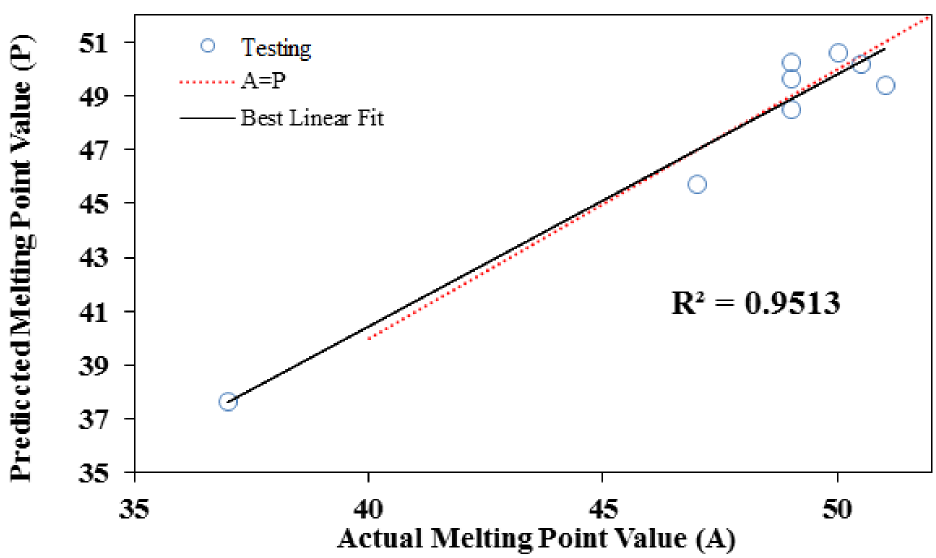
41
39
37
35
35
40
45
50

GA-5-4-1


Testing
A=P
Best Linear Fit
R² = 0.9513
Predicted Melting Point Value (P)
Actual Melting Point Value (A)
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41
39
37
35
35
40
45
50

LM-5-4-1

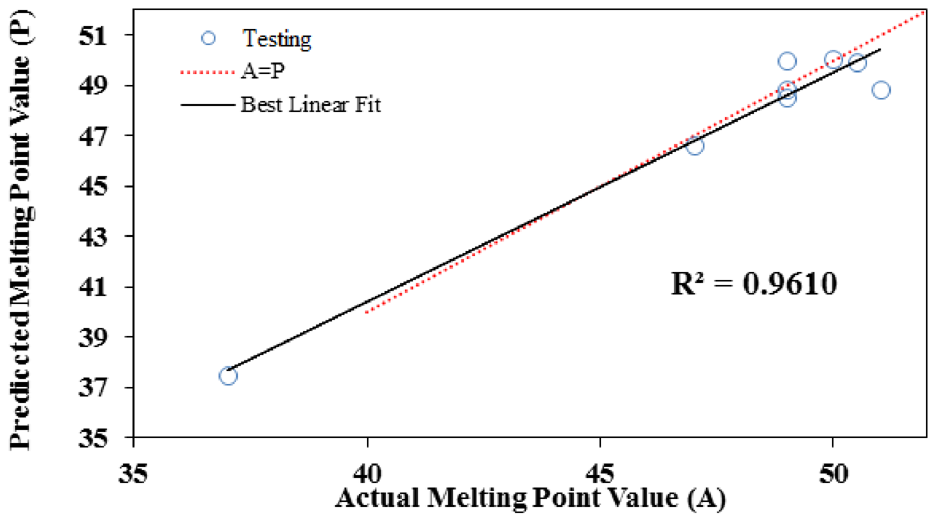
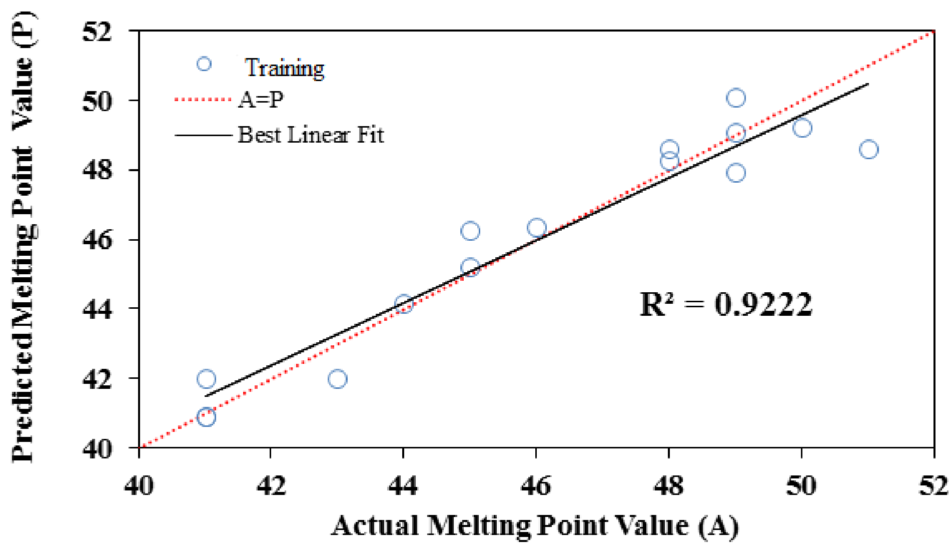
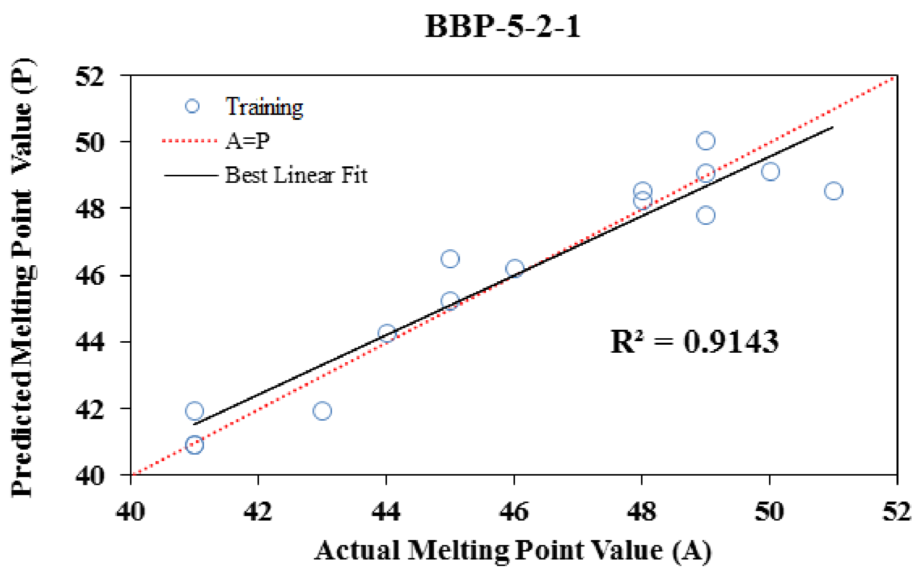


Fig 3:

IBP-5-2-1




BBP-5-2-1
Training
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Predicted Melting Point Value (P)
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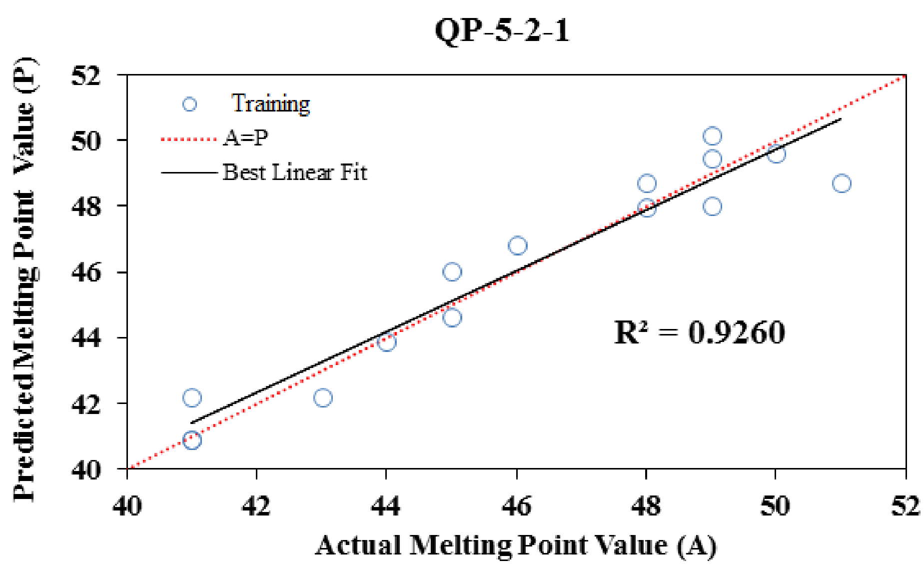
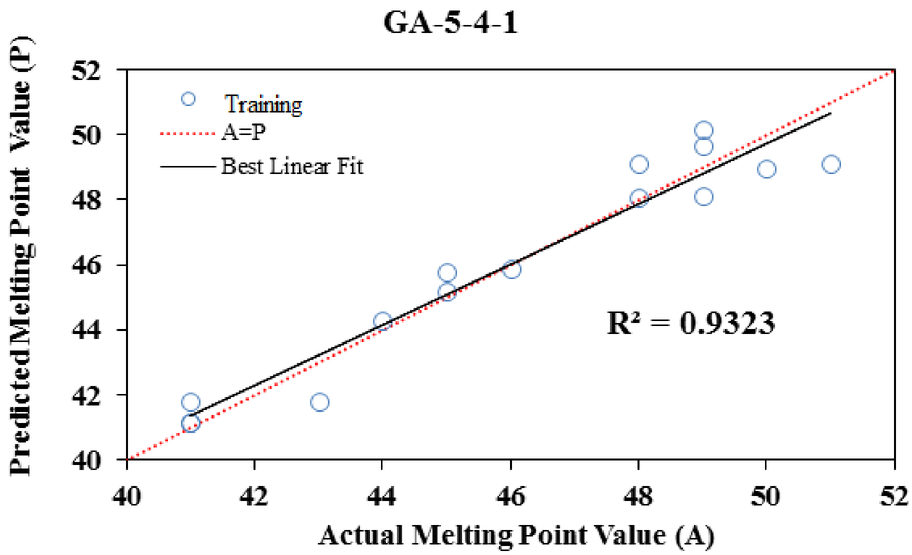
40
42
44
46
48
50
52


QP-5-2-1
Training
A=P
Best Linear Fit
R² = 0.9260
Predicted Melting Point Value (P)
Actual Melting Point Value (A)
40
42
44
46
48
50
52


GA-5-4-1
Training
A=P
Best Linear Fit
R² = 0.9323
Predicted Melting Point Value (P)
Actual Melting Point Value (A)
40
42
44
46
48
50
52

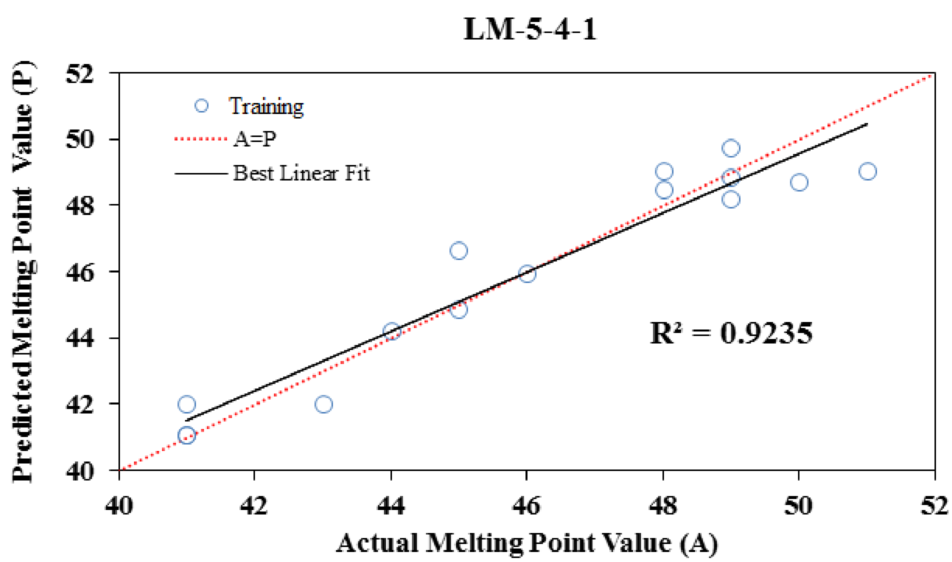

LM-5-4-1
Training
A=P
Best Linear Fit
R² = 0.9235
Predicted Melting Point Value (P)
Actual Melting Point Value (A)
40
42
44
46
48
50
52

Fig 4:

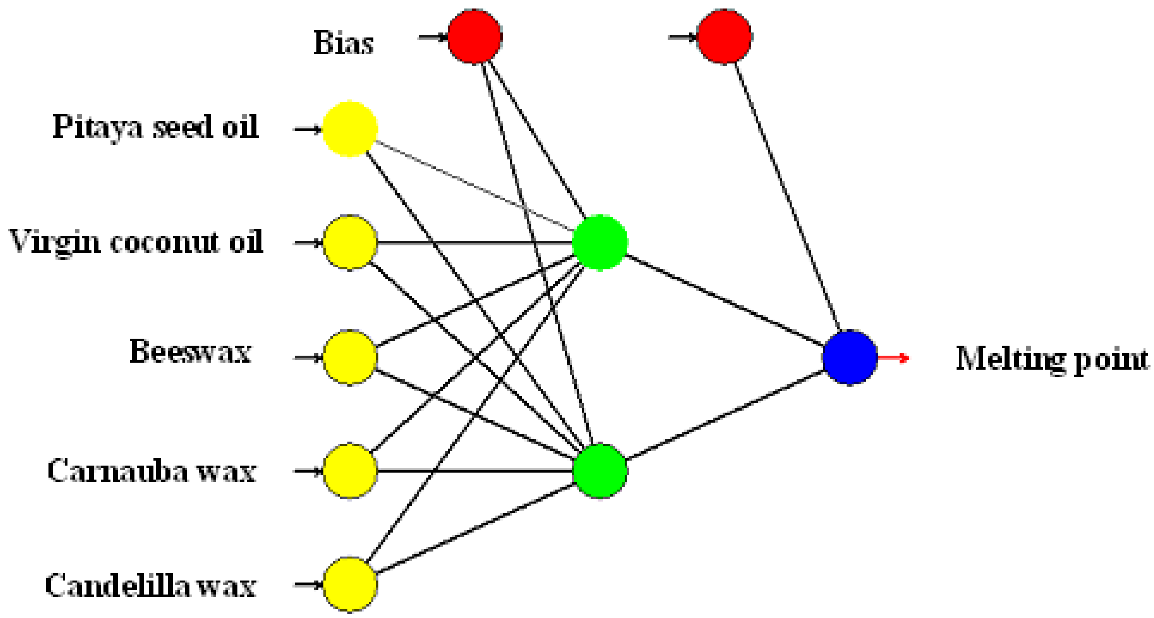

Bias
Pitaya seed oil
Virgin coconut oil
Beeswax
Carnauba wax
Candelilla wax
Melting point

Fig 5:

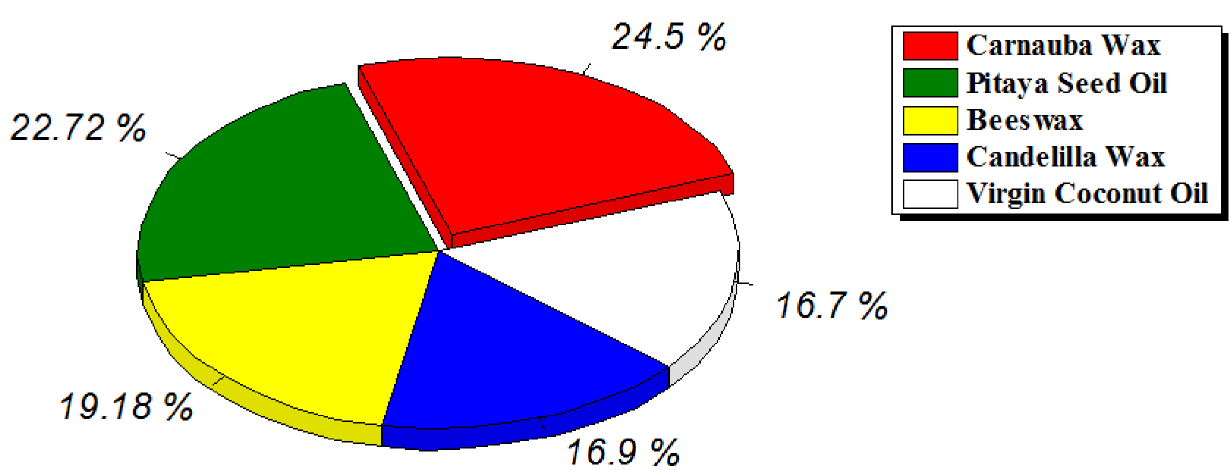

24.5 %
22.72 %
16.7 %
19.18 %
16.9 %
Carnauba Wax
Pitaya Seed Oil
Beeswax
Candelilla Wax
Virgin Coconut Oil

Table list:

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

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

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

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

Table 1.

Run No.	Pitaya seed oil (w/w %)	Virgin coconut oil (w/w %)	Beeswax (w/w %)	Candelilla wax (w/w %)	Carnauba wax (w/w %)	Melting point (ºC)	
						Actual	Predicted
Training Set							
1	35	33.212	8.494	4.997	1.297	41	40.93
2	35	33.212	8.494	4.997	1.297	41	40.93
3	10.185	39.743	25	4.985	3.087	49	50.055
4	22.989	44.847	5.166	5	4.998	44	44.266
5	24.427	29.36	21.11	5	3.102	50	49.123
6	14.997	45	16.945	1.065	4.993	48	48.286
7	10.908	44.982	25	1.11	1	51	48.533
8	26.412	25.6	25	1.001	4.986	49	49.093
9	34.987	33.146	8.289	1.578	5	43	41.96
10	34.966	25	13.85	4.985	4.199	49	47.804
11	17.756	44.997	15.384	3.863	1	46	46.229
12	28.727	25.203	24.993	3.077	1	45	46.527
13	26.866	34.355	18.681	1	2.097	45	45.27
14	34.987	33.146	8.289	1.578	5	41	41.96
15	10.908	44.982	25	1.11	1	48	48.533
Test Set							
1	29	25.203	24.993	3.077	1	47	46.527
2	29	31.964	12.507	4.991	4.993	49	48.622
3	10	40.854	25	2.647	4.42	50	50.056
4	26	25.6	25	1.001	4.986	49	49.093
5	10	45	17.959	4.984	4.986	50.5	49.95
6	29	45	6.345	1.273	1.406	37	37.801
7	19	37.65	19.839	1.977	4.465	51	49.197
8	13	35.326	24.915	4.995	5	49	50.219

Table 2.

Learning algorithm	Architecture	Training data			Testing data		
		RMSE	R^2	AAD	RMSE	R^2	AAD
GA	5-4-1	0.86566	0.9323	1.47838	0.92873	0.9513	1.76428
BBP	5-2-1	0.97687	0.9143	1.55189	0.87029	0.9628	1.41958
LM	5-4-1	0.92512	0.9235	1.51321	0.90478	0.961	1.33627
QP	5-2-1	0.90539	0.90539	1.50871	0.95108	0.9545	1.57108
IBP	5-2-1	0.93064	0.9222	1.47794	0.87405	0.9621	1.45078

Table 3.

Method	Independent Variables					Melting point (ºC)		
	Pitaya seed oil (w/w %)	Virgin coconut oil (w/w %)	Beeswax (w/w %)	Candelilla wax (w/w %)	Carnauba wax (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

Table 4.

Method	Independent Variables					Melting point (ºC)		
	Pitaya seed oil (w/w %)	Virgin coconut oil (w/w %)	Beeswax (w/w %)	Candelilla wax (w/w %)	Carnauba wax (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