

## Extraction optimization of *Quercus cerris* L. wood chips: a comparative study between Full Factorial Design (FFD) and Artificial Neural Network (ANN)

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**Table S1.** Analysis of variance of DPPH, FRAP, TPC, TFC, CTC and HTC methods

**Table S2** Pearson Correlation between yield and the evaluated responses

**Table S3:** Weights and biases of the developed ANN

**Figure S1** Performance of ANN model with different numbers of hidden layers A) 8, B) 9, C) 10, D) 11, and E) 12

**Table S1.** Analysis of variance of DPPH, FRAP, TPC, TFC, CTC and HTC methods

Source	DF	Adj SS	Adj MS	F-Value	P-Value
<b>DPPH scavenging activity</b>					
<b>Model</b>	7	211646	30235	12.90	0.000 *
<b>Linear</b>	3	200264	66755	28.49	0.000 *
Temperature (°C)	1	116327	116327	49.65	0.000 *
Solvent (%EtOH)	1	83936	83936	35.82	0.000 *
Time(h)	1	1	1	0.00	0,984
<b>2-Way Interactions</b>	3	2862	954	0.41	0.750
Temperature (°C)*Solvent (%EtOH)	1	1118	1118	0.48	0.498
Temperature (°C)*Time(h)	1	1339	1339	0.57	0.459
Solvent (%EtOH)*Time(h)	1	405	405	0.17	0.682
<b>3-Way Interactions</b>	1	2793	2793	1.19	0.289
Temperature (°C)*Solvent (%EtOH)*Time(h)	1	2793	2793	1.19	0.289
<b>Error</b>	19	44518	2343		
<b>Total</b>	26	256164			
<b>FRAP</b>					
<b>Model</b>	7	318097	45442	10.05	0.000 *
<b>Linear</b>	3	289690	96563	21.35	0.000 *
Temperature (°C)	1	164633	164633	36.40	0.000 *
Solvent (%EtOH)	1	124568	124568	27.54	0.000 *
Time(h)	1	489	489	0.11	0.746
<b>2-Way Interactions</b>	3	16215	5405	1.19	0.338
Temperature (°C)*Solvent (%EtOH)	1	4696	4696	1.04	0.321
Temperature (°C)*Time(h)	1	5	5	0.00	0.974
Solvent (%EtOH)*Time(h)	1	11514	11514	2.55	0.127
<b>3-Way Interactions</b>	1	6954	6954	1.54	0.230
Temperature (°C)*Solvent (%EtOH)*Time(h)	1	6954	6954	1.54	0.230
<b>Error</b>	19	85940	4523		
<b>Total</b>	26	404037			
<b>TPC</b>					
<b>Model</b>	7	148131	21162	8.16	0.000 *
<b>Linear</b>	3	140430	46810	18.04	0.000 *
Temperature (°C)	1	126270	126270	48.67	0.000 *
Solvent (%EtOH)	1	12271	12271	4.73	0.042 *
Time(h)	1	1889	1889	0.73	0.404
<b>2-Way Interactions</b>	3	343	114	0.04	0.987
Temperature (°C)*Solvent (%EtOH)	1	88	88	0.03	0.856
Temperature (°C)*Time(h)	1	109	109	0.04	0.840
Solvent (%EtOH)*Time(h)	1	146	146	0.06	0.815
<b>3-Way Interactions</b>	1	137	137	0.05	0.821
Temperature (°C)*Solvent (%EtOH)*Time(h)	1	137	137	0.05	0.821

<b>Error</b>	19	49293	2594		
<b>Total</b>	26	197424			
<b>TFC</b>					
<b>Model</b>	7	63538.1	9076.9	10.05	0.000 *
<b>Linear</b>	3	50871.1	16957.0	18.77	0.000 *
<b>Temperature (°C)</b>	1	16551.4	16551.4	18.32	0.000 *
<b>Solvent (%EtOH)</b>	1	20000.7	20000.7	22.14	0.000 *
<b>Time(h)</b>	1	14319.0	14319.0	15.85	0.001 *
<b>2-Way Interactions</b>	3	6258.5	2086.2	2.31	0.109
<b>Temperature (°C)*Solvent (%EtOH)</b>	1	5005.2	5005.2	5.54	0.029 *
<b>Temperature (°C)*Time(h)</b>	1	875.1	875.1	0.97	0.337
<b>Solvent (%EtOH)*Time(h)</b>	1	378.2	378.2	0.42	0.525
<b>3-Way Interactions</b>	1	347.0	347.0	0.38	0.543
<b>Temperature (°C)*Solvent (%EtOH)*Time(h)</b>	1	347.0	347.0	0.38	0.543
<b>Error</b>	19	17162.1	903.3		
<b>Total</b>	26	80700.1			
<b>HTC</b>					
<b>Model</b>	7	874460	124923	15.03	0.000 *
<b>Linear</b>	3	616807	205602	24.73	0.000 *
<b>Temperature (°C)</b>	1	391807	391807	47.13	0.000 *
<b>Solvent (%EtOH)</b>	1	174462	174462	20.99	0.000 *
<b>Time (h)</b>	1	50538	50538	6.08	0.023 *
<b>2-Way Interactions</b>	3	155697	51899	6.24	0.004 *
<b>Temperature (°C)*Solvent (%EtOH)</b>	1	123467	123467	14.85	0.001 *
<b>Temperature (°C)*Time(h)</b>	1	37	37	0.00	0.948
<b>Solvent (%EtOH)*Time(h)</b>	1	32194	32194	3.87	0.064
<b>3-Way Interactions</b>	1	615	615	0.07	0.789
<b>Temperature (°C)*Solvent (%EtOH)*Time(h)</b>	1	615	615	0.07	0.789
<b>Error</b>	19	157959	8314		
<b>Total</b>	26	1032418			
<b>CTC</b>					
<b>Model</b>	7	5848.2	835.46	3.71	0.011 *
<b>Linear</b>	3	5641.1	1880.36	8.36	0.001 *
<b>Temperature (°C)</b>	1	2642.0	2641.96	11.74	0.003 *
<b>Solvent (%EtOH)</b>	1	2999.1	2999.12	13.33	0.002 *
<b>Time(h)</b>	1	0.0	0.00	0.00	0.999
<b>2-Way Interactions</b>	3	263.5	87.83	0.39	0.761
<b>Temperature (°C)*Solvent (%EtOH)</b>	1	69.4	69.37	0.31	0.585
<b>Temperature (°C)*Time(h)</b>	1	8.9	8.91	0.04	0.844
<b>Solvent (%EtOH)*Time(h)</b>	1	185.2	185.22	0.82	0.376
<b>3-Way Interactions</b>	1	5.3	5.30	0.02	0.880
<b>Temperature (°C)*Solvent (%EtOH)*Time(h)</b>	1	5.3	5.30	0.02	0.880

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<b>Error</b>	19	4275.0	225.00
<b>Total</b>	26	10123.2	

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DF, degrees of freedom; SS, sum of squares; MS, mean squares; R<sup>2</sup>, coefficient of determination; DPPH: 2,2-diphenyl-1-picrylhydrazyl expressed as milligrams of Trolox equivalents per gram of dry extract; FRAP: ferric reducing antioxidant power expressed as milligrams of Trolox equivalents per grams of dry extract. TPC: total phenolic content expressed as milligrams of gallic acid per gram of dry extract; TFC: total flavonoid content expressed as milligrams of quercetin equivalents per grams of dry extract; CTC: condensed tannin content expressed as milligrams of tannic acid equivalents per grams of dry extract; HTC: hydrolysable tannins content expressed as milligrams of tannic acid equivalents per grams of dry extract; \* p values lower than 0.05 are statistically significant.

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**Table S2.** Pearson Correlation between yield and the evaluated responses

	Temperature (°C)	TPC (mgGAE/g)	TFC (mgQE/g)	HTC (mgTAE/g)	FRAP (mgTE/g)	DPPH (mgTE/g)
<b>Yield (%)</b>	0.774	0.811	0.787	0.669	0.779	0.791
<b>95%CI</b>	(0.558;0.892)	(0.623;0.910)	(0.581;0.898)	(0.387;0.836)	(0.567;0.894)	(0.587;0.900)

DPPH: 2,2-diphenyl-1-picrylhydrazyl expressed as milligrams of Trolox equivalents per gram of dry extract; FRAP: ferric reducing antioxidant power expressed as milligrams of Trolox equivalents per grams of dry extract. TPC: total phenolic content expressed as milligrams of gallic acid per gram of dry extract; TFC: total flavonoid content expressed as milligrams of quercetin equivalents per grams of dry extract; CTC: condensed tannin content expressed as milligrams of tannic acid equivalents per grams of dry extract; HTC: hydrolysable tannins content expressed as milligrams of tannic acid equivalents per grams of dry extract

**Table S2:** Weights and biases of the developed ANN

<b>Layer 1</b>
b1 = [-3.3658381272721920041; -1.3991178379491064909; 0.73659995576991865729; -0.53182049141105114387; 0.5247235555572924857; -2.9733963321470882057; -0.29085727691318830068; -2.4964822118479084168; -2.8047356204451689976; -3.2135318183290730865];
IW1_1 = [1.3694162100906195345 -4.3091618142965266713 1.1935791040671703822; 2.8121322381007556324 -1.5218647632018840188 0.041052536626025579181; 1.2410943326698309352 4.4725625112068927436 -2.1986119377570134681; 1.7992859703924799497 -0.54371115367242317529 -4.456133682056255374; 1.6843631748729901432 -0.27292574815673481536 3.9010079034444609114; -3.5315655357644906154 0.011234577183720562132 -0.025679126289264435357; -0.95195687849418597626 -2.4057537243378814829 -1.1475221339558825395; -2.210554458180312043 1.7111592469016598805 -0.58368623918766127101; -2.9614786203794487562 0.11948928895135463302 0.17259416977169131369; 0.41276498321934224078 -2.3323459078827615265 1.9361919122015875949];
<b>Layer 2</b>
b2 = [-0.51842244257765668358; -0.66108449055888895973; -0.54882049544378741501];
LW2_1 = [0.94671609759769825843 0.057486181383335541173 0.34417166533069570855 -0.6916455621694962419 -0.74373535304976634563 1.1331329958826239501 -0.8161099264387802199 -0.3444863845680172787 -1.4062761166421580139 -0.7058946673556334428; 1.1952698840557116622 0.13209506421923833397 0.53609279801075515604 -1.1339154431549203217 -1.0731688872653484257 1.0415563925734900863 -0.76866176993251578153 -0.67120669180756709071 -0.9821873938496097356 -0.92983195083105829593; 0.048017442413148953007 0.73243565977217839347 0.38052041677848280621 0.029593823126837982829 0.18298537281625720796 1.2230096454784413762 -0.38715958756250995476 -0.38143242427172541209 -1.1342958393706217279 -0.18005823578382687544];

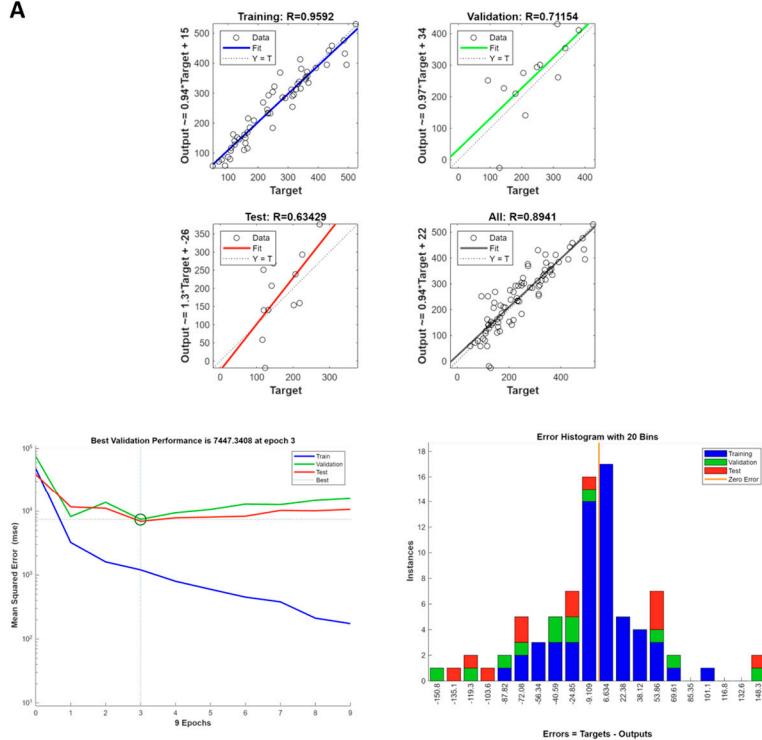
b1: Bias values for hidden layer neurons;

IW1\_1: Weights of synaptic joints between input and hidden layer neurons;

b2: Bias values for hidden layer neurons.

LW2\_1: Weights of synaptic joints between hidden and output layer neurons;

A



Train a neural network to map predictors to continuous responses.

#### Data

Predictors: X - [27x3 double]

Responses: Y - [27x3 double]

X: double array of 27 observations with 3 features.

Y: double array of 27 observations with 3 features.

#### Algorithm

Data division: Random

Training algorithm: Levenberg-Marquardt

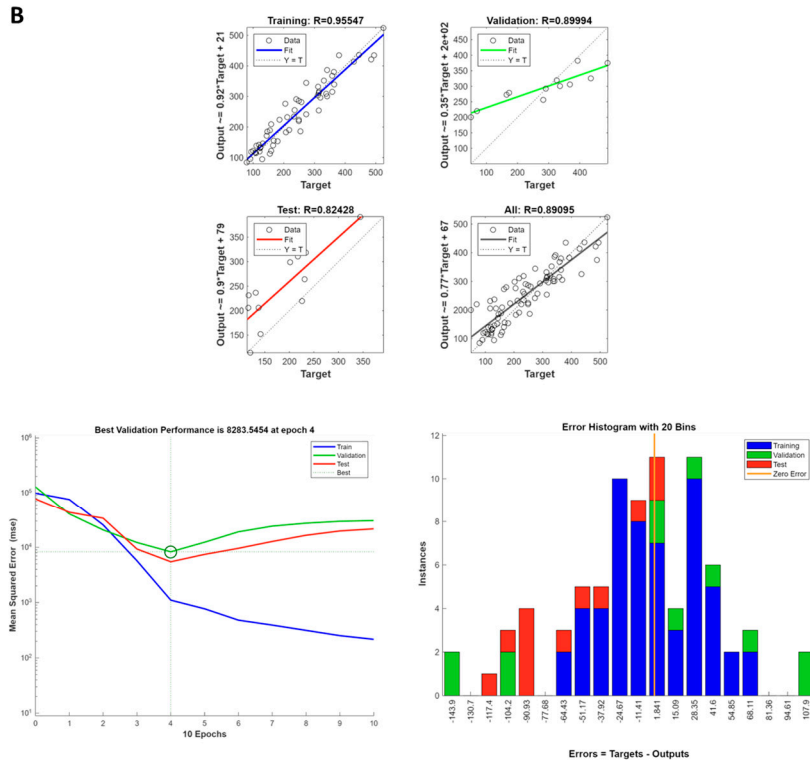
Performance: Mean squared error

#### Training Results

Layer size: 8

	Observations	MSE	R
Training	19	1.2067e+03	0.9592
Validation	4	7.4473e+03	0.7115
Test	4	6.9241e+03	0.6343

B



Train a neural network to map predictors to continuous responses.

#### Data

Predictors: X - [27x3 double]

Responses: Y - [27x3 double]

X: double array of 27 observations with 3 features.

Y: double array of 27 observations with 3 features.

#### Algorithm

Data division: Random

Training algorithm: Levenberg-Marquardt

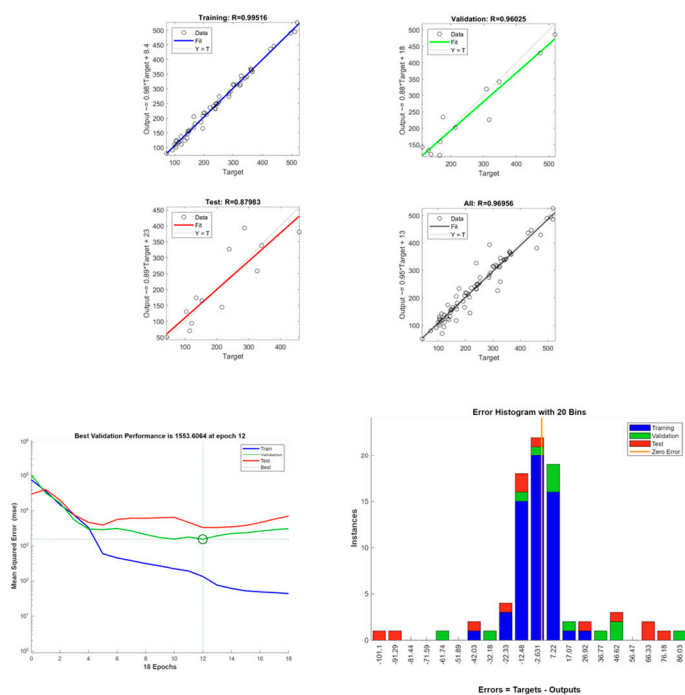
Performance: Mean squared error

#### Training Results

Layer size: 9

	Observations	MSE	R
Training	19	1.1070e+03	0.9555
Validation	4	8.2835e+03	0.8999
Test	4	5.4680e+03	0.8243

C



## Model Summary

Train a neural network to map predictors to continuous responses.

## Data

Predictors:  $x$  - [3x27 double]

Responses:  $y$  - [3x27 double]

$x$ : double array of 27 observations with 3 features.

$y$ : double array of 27 observations with 3 features.

## Algorithm

Data division: Random

Training algorithm: Levenberg-Marquardt

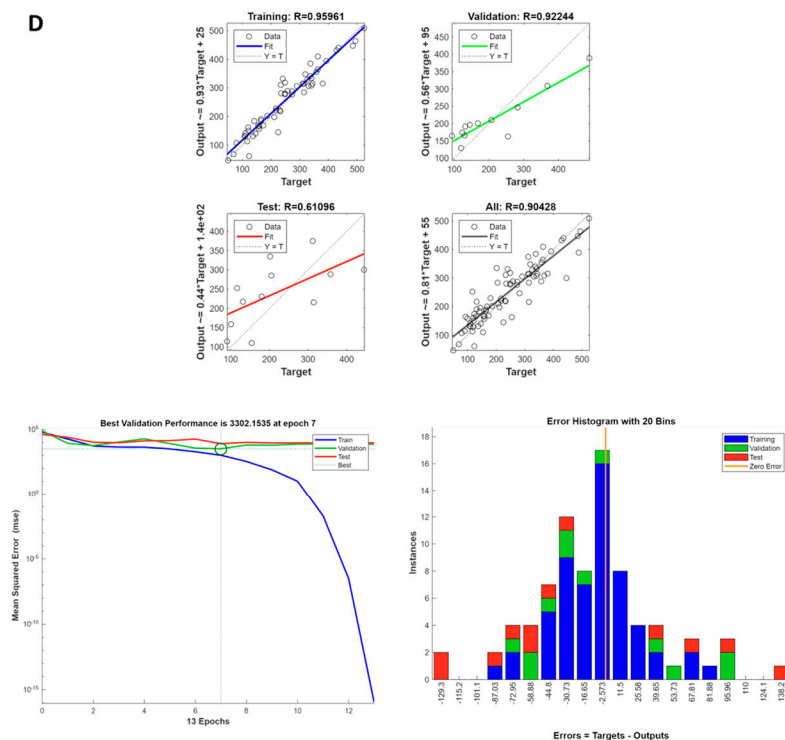
Performance: Mean squared error

## Training Results

Layer size: 10

	Observations	MSE	R
Training	19	134.4447	0.9952
Validation	4	1.5536e+03	0.9603
Test	4	3.3374e+03	0.8798

D



Train a neural network to map predictors to continuous responses.

## Data

Predictors:  $X$  - [27x3 double]

Responses:  $Y$  - [27x3 double]

$X$ : double array of 27 observations with 3 features.

$Y$ : double array of 27 observations with 3 features.

## Algorithm

Data division: Random

Training algorithm: Levenberg-Marquardt

Performance: Mean squared error

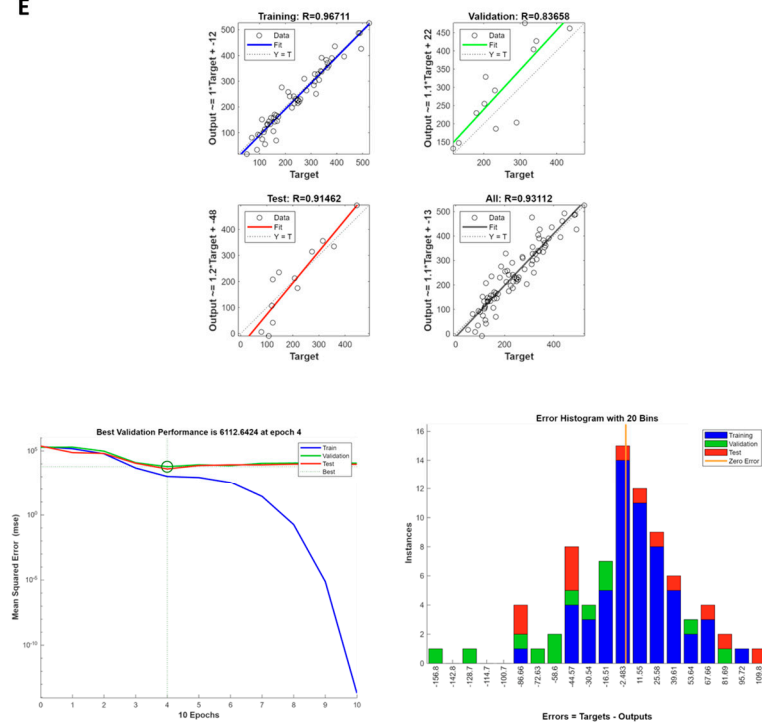
## Training Results

Layer size: 11

	Observations	MSE	R
Training	19	1.0518e+03	0.9596
Validation	4	3.3022e+03	0.9224
Test	4	8.1649e+03	0.6110



E



Train a neural network to map predictors to continuous responses.

#### Data

Predictors: X - [27x3 double]

Responses: Y - [27x3 double]

X: double array of 27 observations with 3 features.

Y: double array of 27 observations with 3 features.

#### Algorithm

Data division: Random

Training algorithm: Levenberg-Marquardt

Performance: Mean squared error

#### Training Results

Layer size:

12

	Observations	MSE	R
Training	19	1.0562e+03	0.9671
Validation	4	6.1126e+03	0.8366
Test	4	4.0670e+03	0.9146

**Figure S1** Performance of ANN model with different numbers of hidden layers A) 8, B) 9, C) 10, D) 11, and E) 12