**Supplementary data sheet**

**Optimization of *Portulaca oleracea* L. extract using response surface methodology and artificial neuronal network and characterization of bioactive compound by high-resolution mass spectroscopy**

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**Table S1: Independent process variables with experimental ranges and levels for heat reflux extraction of *Portulaca oleracea*.**

|  |  |
| --- | --- |
| **Input variables**  | **Variable range and levels (coded)** |
| **unit** | **Code**  | **-α** | **-1** | **0** | **+1** | **+α** |
| Ethanol concentration  | % | X1 | 0 | 25 | 50 | 75 | 100 |
| Time  | min | X2 | 40 | 60 | 90 | 120 | 140 |
| Temperature  | 0C | X3 | 30 | 40 | 50 | 60 | 70 |

**Table S2: Central composite design (CCD) for the independent variables and corresponding response value in RSM and ANN (predicted)**

|  |  |  |
| --- | --- | --- |
| Run  | Independent variables | Responses (predicted) |
| (X1) | (X2) | (X3) | (Y1) | (Y2) |  (Y3) |  (Y4) |
| RSM | ANN | RSM | ANN | RSM | ANN | RSM | ANN |
| 1 | 50 | 140 | 50 | 5.01 | 5.12 | 20.20 | 21.92 | 20.22 | 20.36 | 18.50 | 19.25 |
| 2 | 50 | 40 | 50 | 3.98 | 4.04 | 19.95 | 20.30 | 14.87 | 15.99 | 16.62 | 16.37 |
| 3 | 50 | 90 | 50 | 7.82 | 7.98 | 42.67 | 43.57 | 41.13 | 41.86 | 35.30 | 36.17 |
| 4 | 50 | 90 | 30 | 3.00 | 3.10 | 29.71 | 29.47 | 8.63 | 9.66 | 11.61 | 12.02 |
| 5 | 0 | 90 | 50 | 1.17 | 1.27 | 19.19 | 19.5 | 0.75 | 0.80 | 2.75 | 3.82 |
| 6 | 75 | 60 | 60 | 6.22 | 6.28 | 28.52 | 29.24 | 27.21 | 27.49 | 25.45 | 26.59 |
| 7 | 50 | 90 | 50 | 7.82 | 7.98 | 42.67 | 41.16 | 41.13 | 41.22 | 35.30 | 35.08 |
| 8 | 75 | 120 | 40 | 4.92 | 5.01 | 30.91 | 31.73 | 25.29 | 25.74 | 23.21 | 23.43 |
| 9 | 75 | 60 | 40 | 5.23 | 5.11 | 31.87 | 32.86 | 23.92 | 21.62 | 22.49 | 22.73 |
| 10 | 25 | 120 | 60 | 4.86 | 5.01 | 26.23 | 25.12 | 19.65 | 21.59 | 16.96 | 17.24 |
| 11 | 50 | 90 | 50 | 7.82 | 7.98 | 42.67 | 43.16 | 41.13 | 40.22 | 35.30 | 35.08 |
| 12 | 100 | 90 | 50 | 5.83 | 5.63 | 31.74 | 31.74 | 29.36 | 30.56 | 26.04 | 25.41 |
| 13 | 50 | 90 | 50 | 7.82 | 7.98 | 42.67 | 43.84 | 41.13 | 41.92 | 35.30 | 35.52 |
| 14 | 75 | 120 | 60 | 6.97 | 6.97 | 29.69 | 29.71 | 31.01 | 29.65 | 28.18 | 27.55 |
| 15 | 25 | 60 | 60 | 3.31 | 3.91 | 24.96 | 24.29 | 14.59 | 15.03 | 15.42 | 15.87 |
| 16 | 50 | 90 | 70 | 5.68 | 5.56 | 30.66 | 31.54 | 22.28 | 22.85 | 21.58 | 22.27 |
| 17 | 25 | 60 | 40 | 2.68 | 2.71 | 22.79 | 23.16 | 6.67 | 8.02 | 10.42 | 11.08 |
| 18 | 50 | 90 | 50 | 7.82 | 8.01 | 42.67 | 43.23 | 41.13 | 42.05 | 35.30 | 35.06 |
| 19 | 50 | 90 | 50 | 7.82 | 7.89 | 42.67 | 43.59 | 41.13 | 42.15 | 35.30 | 36.16 |
| 20 | 25 | 120 | 40 | 3.18 | 3.06 | 21.93 | 21.05 | 9.30 | 9.01 | 9.95 | 10.02 |

 X1: Ethanol concentration (%); X2: time (h); X3: temperature (0C); TPC: total phenolic content (mgGAE/g); TFC: total flavonoid content (mgCAE/g); DPPH: DPPH-radical scavenging activity (% inhibition); FRAP: ferric reducing antioxidant power (µM ascorbic acid equivalent).

**Table S3: Experiment data of the validation of predicted values at optimal extraction conditions of areal parts of *Portulaca oleracea*.**

**Optimal condition:** X1: Ethanol concentration (%): 60%; X2: time (min): 90.5; X3: temperature (0C): 50.

|  |  |  |
| --- | --- | --- |
| **Dependent variables**  | **Experimental value**  | **Predicted value** |
| TPC (mgGAE/g) | 8.23 ± 1.06 | 8.12 |
| TFC (mgCAE/g) | 43.12 ± 1.15 | 43.23 |
| DPPH (% inhibition) | 43.01 ± 1.25 | 42.98 |
| FRAP (µM) | 35.98 ± 0.19 | 36.81 |

TPC: total phenolic content (mgGAE/g); TFC: total flavonoid content (mgCAE/g); DPPH: DPPH-radical scavenging activity (% inhibition); FRAP: ferric reducing antioxidant power (µM ascorbic acid equivalent).



**Figure S1: Pareto chart for the extraction of polyphenols and antioxidants from the aerial part of *Portulaca oleracea* (APO) using heat reflux extraction (HRE).**