GC-MS Fingerprinting Combined with Chemometric Methods Reveals Key Bioactive Components in Acori Tatarinowii Rhizoma

Wenbin Liu , Bingyang Zhang , Zhongquan Xin , Dabing Ren and Lunzhao Yi \*

**Table S1.** The qualitative and quantitative results of essential oils from ATR.

**Listed in ijms-200069-Supplementary materials.**

**Table S2.** Overview of the experimental and predicted DPPH values for PLSR model after outlier elimination

|  |  |  |  |
| --- | --- | --- | --- |
| **Sample ID** | **Ym** | **YP** | **RE(%)** |
| 1 a | 11.597 | 13.321 | 14.86 |
| 2 a | 15.260 | 15.134 | -0.82 |
| 3 a | 25.038 | 24.777 | -1.04 |
| 4 a | 28.190 | 27.317 | -3.10 |
| 5 a | 12.712 | 14.771 | 16.20 |
| 7 a | 24.102 | 22.859 | -5.16 |
| 8 a | 25.209 | 25.002 | -0.82 |
| 10 a | 22.491 | 18.236 | -18.92 |
| 12 a | 22.183 | 27.653 | 24.66 |
| 13 a | 24.977 | 26.610 | 6.54 |
| 14 a | 40.243 | 40.321 | 0.19 |
| 15 a | 21.406 | 20.171 | -5.77 |
| 16 a | 21.188 | 19.169 | -9.53 |
| 17 a | 19.337 | 22.516 | 16.44 |
| 18 a | 20.269 | 21.570 | 6.42 |
| 19 a | 29.292 | 28.176 | -3.81 |
| 20 a | 28.729 | 27.660 | -3.72 |
| 21 a | 26.409 | 23.337 | -11.64 |
| 22 a | 22.655 | 25.319 | 11.76 |
| 23 a | 39.761 | 40.787 | 2.58 |
| 26 a | 23.224 | 22.842 | -1.64 |
| 29 a | 25.284 | 21.874 | -13.49 |
| 33 a | 25.524 | 28.778 | 12.75 |
| 34 a | 25.279 | 29.189 | 15.46 |
| 36 a | 41.826 | 40.145 | -4.02 |
| 39 a | 41.995 | 38.075 | -9.33 |
| 40 a | 38.966 | 40.410 | 3.71 |
| 41 a | 19.524 | 19.293 | -1.19 |
| 42 a | 21.800 | 21.974 | 0.80 |
| 43 a | 30.243 | 25.931 | -14.26 |
| 44 a | 29.503 | 28.709 | -2.69 |
| 45 a | 18.426 | 20.897 | 13.41 |
| 46 a | 20.013 | 20.151 | 0.69 |
| 47 a | 18.233 | 17.913 | -1.76 |
| 6 b | 14.962 | 15.434 | 3.15 |
| 9 b | 29.259 | 24.554 | -16.08 |
| 11 b | 20.894 | 18.726 | -10.37 |
| 24 b | 26.062 | 21.727 | -16.63 |
| 25 b | 23.370 | 22.706 | -2.84 |
| 27 b | 24.741 | 22.625 | -8.55 |
| 28 b | 24.714 | 22.336 | -9.62 |
| 30 b | 17.636 | 22.887 | 29.77 |
| 35 b | 41.268 | 39.693 | -3.82 |

a: sample in the calibration set; b: sample in the validation set; Ym: measured DPPH values; YP: predicted DPPH values; RE: relative error.