Analysis Of Common Volatile Constituents Between Herbal Pair Ephedra Sinica Stapf-zingiber Officinale Rosc And Its Single Herb By Gc-ms Combined With Amwfa Method

Corresponding Author:
Prof. Xiao-Ru Li,
PROFESSOR, Research Center of Modernization of Chinese Medicine, Central South University, 410083 - China

Submitting Author:
Ms. Shuai-Hua Chen,
Lecturer, College of Chemistry and Chemical Engineering, Jiangxi Normal University of Science and Technology, 330013 - China

Article ID: WMC001071
Article Type: Original Articles
Article URL: http://www.webmedcentral.com/article_view/1071
Subject Categories: CHINESE MEDICINE
Keywords: Herbal pair Ephedra sinica Stapf-Zingiber officinal Rosc, GC-MS, alternative moving window factor analysis, Temperature-programmed retention indices (PTRIs), volatile oil, common constituents

How to cite the article: Chen S, Li X. Analysis Of Common Volatile Constituents Between Herbal Pair Ephedra Sinica Stapf-zingiber Officinale Rosc And Its Single Herb By Gc-ms Combined With Amwfa Method.
WebmedCentral CHINESE MEDICINE 2010;1(10):WMC001071

Source(s) of Funding:
This work is financially supported by the National Nature Foundation Committee of PR China (Grant Nos.20235020 and 20475066) and the Cultivation Fund of Key Scientific and Technical Innovation Project, Ministry of Education of China (No. 704036).
Analysis Of Common Volatile Constituents Between Herbal Pair Ephedra Sinica Stapf-zingiber Officinal Rosc And Its Single Herb By Gc-ms Combined With Amwfa Method

Author(s): Chen S , Li X

Abstract

Analysis of common volatile constituents between herbal pair (HP) Ephedra sinica Stapf (ESS)-Zingiber officinal Rosc (ZOR)and its single herb was performed by the method of GC-MS and alternative moving window factor analysis (AMWFA). Identification of the compounds was also assisted by comparison of temperature-programmed retention indices (PTRIs) on the OV-1 column with authentic samples. AMWFA analysis indicates that there are 13 common volatile constituents in HP ESS-ZOR and single herb ESS, and 36 common volatile constituents in HP ESS-ZOR and single herb ZOR, and 5 common volatile constituents among these three systems, and volatile chemical components in HP ESS-ZOR are mainly from single herb ZOR.

Introduction

The compatibility of Ephedra sinica Stapf (ESS) with Zingiber officinal Rosc (ZOR) either enhances efficacy of the medicine or reduces noxious side effect of the medicine, which could improves clinical curative effects [1]. ESS has the effects of diaphoretics pungent in flavor and warm in property, gently clear floating upward, which is the first medicine of relieving exterior syndromes by dispelling pathogenic wind, and ZOR has the effects of diaphoretics pungent in flavor and warm in property, and powerful force of the diaphoresis. The compatibility of ESS-ZOR has the effects of relieving exterior syndromes by dispelling pathogenic wind, promoting skin eruption by dispelling pathogens, and arresting bleeding. These two herbal medicines are often used together for affection by exopathogenic wind-cold shown as aversion to cold, fever, headache and anhidrosis to expel exogenous pathogenic factors and relieving exterior syndrome. Essential oil of the recipe has the anti-inflammatory effect[2],but its chemical components have not been reported yet.

The aim of this research work is at systematically investigating of the volatile chemical components of ESS, ZOR, and the HP by the method of gas chromatography—mass spectrometry (GC-MS) and alternative moving window factor analysis (AMWFA) [3,4] , and then carrying out qualitative and quantitative analysis between HP and its single herbal medicines, i.e. ESS, ZOR, by means of chemometric techniques and temperature-programmed retention indices (PTRIs). By comparison analysis, the differences and the sameness of volatile components between the recipe and its single herbal medicines can be gotten, and a further knowledge about the mechanism of changes of the chemical components in herbal pairs (two herbal medicines used together) can be obtained. To our best knowledge, it is the first report on the volatile components of the recipe. The application of PTRIs has greatly improved the accuracy of qualitative analysis.

Generally speaking, the analysis of volatile oil is usually conducted with GC–MS, which contributed greatly to the characterization and identification of volatile chemical components in complex systems. However, it is difficult to assess the purity of chromatographic peaks by general GC and the peak inspected as one component may be mixture of several components, because the boiling points of compounds are close to each other, then co-elution of two or more different compounds is very possible. For these overlapping peaks, it is hard to identify the component and even possible to lead to wrong conclusion by direct searches in MS database alone, and it would be also difficult to determine the area of each component in them.

Furthermore, temperature-programmed retention index (PTRI) [5-6] is also employed to the identification of compound. Richmond [7-9] thought that IuT can be highly reproducible on a given capillary column, whose stationary phase is fixed, if working variables, such as carrier flow-rate, film thickness and linear temperature programming rate are standardized. For those substances whose mass spectra are similar to each other, the identification is difficult by directly mass spectral searching alone. However, they have different retention times, from which the qualitative results can
be confirmed and determined. Therefore, by using PTRIs, the identification of the compound will be more accurate to some extent. The combination of PTRIs and chemometric techniques can greatly improve the identification of chemical components in volatile oils of herbal medicines.

**Methods**

2.1 Extraction of essential oil

Single herbal medicines ESS and ZOR were purchased from Jiuzhitang medical materials corporation (Changsha, Hunan, China), and they were both identified by Institute of Materia Medica, Hunan Academy of Traditional Chinese Medicine and Materia Medica (Changsha, Hunan, China). n-Alkane standard solutions of C8–C20 (mixture no. 04070) and C21–C40 (mixture no. 04071) were purchased from Fluka Chemika.

Extraction of essential oil of the recipe: 100g of dried powder of each single herbal medicine, HS and RS, were weighted exactly and mixed and then processed according to the standard method described in Chinese Pharmacopoeia (2000 version) [10].

Extraction of essential oil of single herbal medicine was carried out by the same method as mentioned above.

2.2 Instruments and experimental conditions

The GC-MS instrument was QP2010 with OV-1 capillary column (30mm x0.25mm I.D.). In analysis, the column temperature was set at 40° initially, which was then increased to 120° at a rate of 2°/min and finally to 230° at a rate of 10°/min (maintained for 15 min). The inlet temperature was kept at 250° and interface temperature at 280°. The carrier gas was Helium with a constant flow-rate of 1.0ml/min. To the experimental conditions of the mass spectrometer, electron impact (EI+) mass spectra were recorded at 70 eV. Ionization energy in full scan model was in the ranges of 20−400 amu with 3.8 scan/s. The ionization source temperature was set at 230°.

2.3 Retention indices

Van Den Dool and Dec Kratz [11] proposed a quasi-linear equation for temperature-programmed retention indices as follows (Eq. 1):

$$I_uT = 100 \times \frac{n+(tu-tn)/(tn+1-tn)}{n}$$

where $I_uT$ is the temperature-programmed retention index of the interest, $tn$, $tn+1$, $tu$ are the retention time in minutes of the two standard $n$-alkanes containing $n$ and $n+1$ carbons of the interest, respectively. This equation was used to calculate retention indices in the research work.

2.4 Data analysis

Data analysis were performed on a Pentium based IBM compatible personal computer, and all programs of chemometric resolution methods were coded in MATLAB 6.5 for windows, and all the calculations were performed on a Pentium IV processor based IBM compatible personal computer. Resolved spectra were identified by matching with the standard mass spectral database of the National Institute of Standards and Technology (NIST).

**Results and discussion**

3.1 Resolution of overlapped peaks by AMWFA

For the sake of resolving the overlapping peaks, many chemometric methods, such as evolving factor analysis (EFA) [12,13], windows factor analysis (WFA) [14-16], heuristic evolving latent projections (HELP) [17-19], sub window factor analysis (SFA) [20-22], evolving window orthogonal projection (EWOP) [23-24], and evolving sub window comparison (ESC) [24], have been developed to provide more information for chemical analysis both in chromatographic separation and in spectral identification, which make it possible to extract “pure” spectra from complex chromatograms. These methods can achieve the true solution successfully but can’t extract “pure” spectra for the embedded peaks and therefore determine the number of common components in different samples rapidly. In order to solve this problem, a new proposed chemo metric method, named alternative moving window factor analysis (AMWFA) [25], was introduced. AMWFA is the extension and combination of multi-component spectral correlation chromatography (MSCC) [26] and sub window factor analysis (SFA) [20-22]. This method could use the cross-information hidden in two systems to determine the number of common components in different samples and then to identify their corresponding spectra of common components automatically.

The total ion chromatograms (TIC) of herbal medicines ESS (A), ZOR (B) and the HP (C) are shown in Fig.1, respectively. To illustrate how to extract the pure mass spectra efficiently, the peak clusters marked X (30.365−31.446min) and Y (30.364−30.964min) are picked out as examples and then processed by AMWFA.

Here, peak cluster X is taken as the base matrix, and peak cluster Y as the target matrix. First, MSCC and inverse projection MSCC (IP-MSCC) are employed to see whether the two peak clusters contain common components in different samples and then to identify their corresponding spectra of common components automatically.

The total ion chromatograms (TIC) of herbal medicines ESS (A), ZOR (B) and the HP (C) are shown in Fig.1, respectively. To illustrate how to extract the pure mass spectra efficiently, the peak clusters marked X (30.365−31.446min) and Y (30.364−30.964min) are picked out as examples and then processed by AMWFA.
shown in Fig.2, which indicates that the mass spectra features of the compounds in peak cluster X are highly correlated with that in peak cluster Y and then the two peak clusters contain common components. The result obtained by common rank analysis (Fig.3) shows clearly that the number of common components in the two peak clusters is 3, because the first three values (No.1, No.2 and No.3) on the Y axis are almost zero, and the values after No.4 on the Y axis become on the increase gradually. At the same time, we can also obtain the common rank map and spectral auto-correlative curves by AMWFA, as shown in Fig.4 (A) and (B).

Resolution of pure mass spectra for components are followed to conduct after the number of common components in the two systems, i.e. perk cluster X and perk cluster Y, has been obtained. According to AMWFA, on the region in which the number of common components is equal to one, the corresponding pure mass spectrum could be acquired from the eigenvector. We take the range 5-40 of X as the base matrix, and then the moving window searching was conducted on the range 18-165 of Y with a fixed window size 2, then we can obtain the common rank map as shown in Fig.4 (A). During the process of moving window scanning, the mass spectra and the similarity between the two close mass spectra were obtained by calculation with formula. The spectral auto-correlative curve was also acquired, as shown Fig.4 (B), by plotting of similarity vs retention time. In Fig.4 (A), we can see clearly that there are three regions (48-150,152-179,190-228), in which the number of common components is close to 1, in the common rank map, and three flat regions (indicated by R1, R2 and R3 in Fig.4 (B)) with similarity being close to 1 appear in the corresponding spectral auto-correlative curve. If the number of common components is equal to 1, a pure spectrum can be acquired from the corresponding region with correlation coefficient close to 1 in the spectral auto-correlative curve. In the Fig.4 (B), three flat parts indicated by R1, R2 and R3 show the regions, in which the three identified mass spectra were picked out. By matching search from NIST107 standard mass spectral database, the resolution result by AMWFA shows the three common components in peak clusters X and Y are [E]-3(10)-caren-2-ol(R1), 3,7-dimethyl-1,6-octadien-3-ol (R2), and 3,7-dimethyl-1,6-octadienal (R3) respectively, with the match similarity of 0.9160, 0.9850 and 0.9705. The pure chromatograms of peak clusters X and Y are showed in Fig.8 and Fig.9 which indicates that both peak clusters X and Y are overlapping ones of three components Fig.5, Fig.6 and Fig.7 shows their resolved mass spectra. In Fig.5, Fig.6 and Fig.7, a, b and c were standard mass spectra of R1, R2 and R3, respectively.

3.2 Quantitative analysis of volatile components
The overall volume integration method [22-24] was used for all the chromatogram peaks in order to obtain the quantitative results of each component. In total, 43, 59, and 67 volatile active components in volatile oil of ESS, ZOR, and HP were respectively determined qualitatively and quantitatively, accounting for 77.85%, 66.51% and 87.54% total contents of volatile oil of ESS, ZOR and HP respectively. Their relative content and retention indices (RI) are given in Table 1, where the components are listed in order of elution on the OV-1 column.

3.3 Comparison of volatile components between the HP and single herbs
From Table 1, the main volatile chemical components are are α, α,4-trimethyl-3-cyclohexene-1-methanol/C10H18O (31.9%), n-hexadecanoic acid (6.36%), D-limonene(3.95%),4-(1-methylethyl)-1-cyclohexene-1-carboxaldehyde (3.08%), 1-methyl-3-(1-methylethyl)-benzene (2.27%) for ESS, and camphene(6.4%),(E)-3,7-dimethyl-2,6-Octadien-1-ol (4.77%), α-farnesene (4.13%), [s-(R@,s@)]-3-(1,5-dimethyl-4-hexenyl)-6-methylene-cyclohexene(4.09%), α-pinene (3.22%), α, α,4-trimethyl-3-cyclohexene-1-methanol(3.15%) for ZOR, and β-phellandrene (16.33%), camphene(11%), α, α,4-trimethyl-3-cyclohexene-1-methanol (6.06%), [s-[R,s@]]-3-(1,5-dimethyl-4-hexenyl)-6-methylene-cyclohexene (4.33%), α, farnesene(4.17%), borneol(4.1%), α-pinene(3.4%) for the HP. Compared with HP, 28 and 23 chemical components disappeared in the essential oil of the ESS and ZOR respectively, such as D-Limonene and dodecanolic acid from ESS, 2-Heptanone and 3,7-dimethyl-2-octen-1-ol from ZOR. Meanwhile, 23 new chemical components, such as 2-decanol and bornyl acetate, appeared in the essential oil of HP. Especially, the content of main component, α, α, 4-trimethyl-3-cyclohexene-1-methanol in ESS was only 6.06% in the HP.

This is based on some chemical reactions taking place during the process of decocting two single herbs, which usually include oxidation, reduction, condensation, and especial hydrolysis. In addition to chemical reactions, much attention should be paid to physical effects like solubilization effect and co-dissolving effect in decoction of two single herbs, which is very popular in traditional Chinese medicinal prescriptions.
Conclusions

In this paper, the essential oils of the herb pair and two single herbs ESS and ZOR have been investigated for the first time. By applying chemometric method upon two-dimensional data together with PTRIs, three essential oil samples from the recipe, and two single herbs ESS and ZOR were analyzed and compared regarding their qualitative and relatively quantitative characteristics. The information about the chemical constituents of essential oils is useful and necessary to the further pharmacological study of the recipe ESS-ZOR, which will certainly help us to utilize the recipe ESS-ZOR better. It is worthy noting that the application of AMWFA to the characterization of the components of essential oils is more convenient for the comprehensive comparison between the complex systems. In addition, the results obtained showed that the accuracy of qualitative analysis could be greatly enhanced by the combination of PTRIs. The strength of the chemometric techniques assisted with PTRIs in obtaining more information from the GC–MS data is demonstrated in this investigation.

References


Acknowledgement(s)

This work is financially supported by the National Nature Foundation Committee of PR China (Grant Nos.20235020 and 20475066) and the Cultivation Fund of Key Scientific and Technical Innovation Project, Ministry of Education of China (No. 704036).
Illustrations

Illustration 1

Fig. 1 TIC curves of volatile oils of ESS (A), ZOR (B) and HP ESS-ZOR (C)
Illustration 2

Fig.2 Results of obtained by MSCC and IP-MSCC analysis
Illustration 3

Fig. 3 Results of common rank analysis
Illustration 4

Fig. 4 Resolution results A: Common rank map from AMEFA; B: spectral auto-correlative curves from AMWFA
Illustration 5

Fig. 5 Standard mass spectrum (a) and resolved mass spectrum (b) of [E]-3(10)-caren-2-ol
Illustration 6

Fig. 6 Resolved mass spectrum (a) and standard mass spectrum (b) of 3,7-dimethyl-1,6-octadien-3-ol
Illustration 7

Fig. 7 Resolved mass spectrum (a) and standard mass spectrum (b) of 3,7-dimethyl-1,6-octadienal
Illustration 8

Fig. 8 Resolved chromatograms of peak cluster X (1-R1, 2-R2, 3-R3)
Illustration 9

Fig. 9 Resolved chromatograms of peak cluster Y (1-R1, 2-R2, 3-R3)
Main chemical components of volatile oil from ESS, ZOR and ESS-ZOR

<table>
<thead>
<tr>
<th>No.</th>
<th>Component/molecular formula</th>
<th>ESS (rc)</th>
<th>ZOR (rc)</th>
<th>ESS-ZOR (rc)</th>
<th>Average RI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2-Heptanone/C\textsubscript{7}H\textsubscript{14}O</td>
<td>——</td>
<td>0.08</td>
<td>——</td>
<td>854.324</td>
</tr>
<tr>
<td>2</td>
<td>2-Heptanol/C\textsubscript{7}H\textsubscript{16}O</td>
<td>——</td>
<td>0.24</td>
<td>0.26</td>
<td>875.171</td>
</tr>
<tr>
<td>3</td>
<td>1,7,7-trimethyl-Tricyclo[2.2.1.0\subscript{2,6}]heptane/C\textsubscript{10}H\textsubscript{16}</td>
<td>——</td>
<td>0.48</td>
<td>0.24</td>
<td>906.470</td>
</tr>
<tr>
<td>4</td>
<td>α-Pinene/C\textsubscript{10}H\textsubscript{16}</td>
<td>——</td>
<td>3.22</td>
<td>3.40</td>
<td>919.750</td>
</tr>
<tr>
<td>5</td>
<td>Camphene/C\textsubscript{10}H\textsubscript{16}</td>
<td>——</td>
<td>6.40</td>
<td>11.00</td>
<td>936.145</td>
</tr>
<tr>
<td>6</td>
<td>(1S)-6,6-dimethyl-2-methylene-Bicyclo[3.1.1]heptane/C\textsubscript{10}H\textsubscript{16}</td>
<td>——</td>
<td>——</td>
<td>0.08</td>
<td>953.971</td>
</tr>
<tr>
<td>7</td>
<td>β-Myrcene/C\textsubscript{10}H\textsubscript{16}</td>
<td>——</td>
<td>2.74</td>
<td>1.11</td>
<td>975.501</td>
</tr>
<tr>
<td>8</td>
<td>α-Phellandrene/C\textsubscript{10}H\textsubscript{16}</td>
<td>——</td>
<td>1.58</td>
<td>0.70</td>
<td>985.098</td>
</tr>
<tr>
<td>9</td>
<td>1-methyl-4-(1-methylethyl)-7-Oxabicyclo[2.2.1.1]heptane/C\textsubscript{10}H\textsubscript{18}O</td>
<td>0.72</td>
<td>——</td>
<td>——</td>
<td>997.853</td>
</tr>
<tr>
<td>No.</td>
<td>Compound Name</td>
<td>Molecular Formula</td>
<td>Alpha</td>
<td>Beta</td>
<td>R Value</td>
</tr>
<tr>
<td>-----</td>
<td>-----------------------------------------------</td>
<td>-------------------</td>
<td>-------</td>
<td>-------</td>
<td>----------</td>
</tr>
<tr>
<td>17</td>
<td>tetramethyl-Pyrazine</td>
<td>C_{10}H_{18}N_{2}</td>
<td>1.20</td>
<td>—</td>
<td>0.21</td>
</tr>
<tr>
<td>18</td>
<td>2-Nonanone</td>
<td>C_{9}H_{18}O</td>
<td>—</td>
<td>0.38</td>
<td>0.20</td>
</tr>
<tr>
<td>19</td>
<td>methyl(1-methylethenyl)-Benzene</td>
<td>C_{10}H_{12}</td>
<td>0.55</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>20</td>
<td>2-Decanol</td>
<td>C_{10}H_{22}O</td>
<td>—</td>
<td>—</td>
<td>0.31</td>
</tr>
<tr>
<td>21</td>
<td>1,3,3-trimethyl-Bicyclo[2.2.1]heptan-2-ol</td>
<td>C_{10}H_{16}O</td>
<td>—</td>
<td>—</td>
<td>0.12</td>
</tr>
<tr>
<td>22</td>
<td>trans-1-methyl-1-(1-methylethyl)-2-Cyclohexen-1-ol</td>
<td>C_{10}H_{18}O</td>
<td>—</td>
<td>0.52</td>
<td>0.49</td>
</tr>
<tr>
<td>23</td>
<td>(1R)-1,7,7-trimethyl-Bicyclo[2.2.1]heptan-2-one</td>
<td>C_{10}H_{16}O</td>
<td>—</td>
<td>0.38</td>
<td>0.18</td>
</tr>
<tr>
<td>24</td>
<td>cis-1-methyl-1-(1-methylethyl)-2-Cyclohexen-1-ol</td>
<td>C_{10}H_{18}O</td>
<td>—</td>
<td>—</td>
<td>0.28</td>
</tr>
<tr>
<td>25</td>
<td>5-methyl-2-(1-methylethyl)-Cyclohexanone</td>
<td>C_{10}H_{18}O</td>
<td>0.96</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>26</td>
<td>(R)-3,7-dimethyl-6-Octenal</td>
<td>C_{10}H_{18}O</td>
<td>—</td>
<td>0.05</td>
<td>—</td>
</tr>
<tr>
<td>27</td>
<td>Borneol</td>
<td>C_{10}H_{18}O</td>
<td>—</td>
<td>1.23</td>
<td>4.10</td>
</tr>
<tr>
<td>28</td>
<td>4-(1-methylethyl)-2-Cyclohexen-1-one</td>
<td>C_{9}H_{14}O</td>
<td>0.03</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td>Chemical Formula</td>
<td>Concentration</td>
<td>Retention Time</td>
<td>Molecular Weight</td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>--------------------------</td>
<td>---------------</td>
<td>----------------</td>
<td>------------------</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>3,7-dimethyl-2-Octen-1-ol/C_{10}H_{20}O</td>
<td>0.54</td>
<td></td>
<td>1212.860</td>
<td></td>
</tr>
<tr>
<td>33</td>
<td>Benzylidenemalonaldehyde/C_{10}H_{8}O_{2}</td>
<td>0.03 0.14</td>
<td></td>
<td>1215.287</td>
<td></td>
</tr>
<tr>
<td>34</td>
<td>[E]-3(10)-caren-2-ol/ C_{10}H_{16}O</td>
<td>0.60 0.60</td>
<td></td>
<td>1228.954</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>[\pm/-]-3,7-dimethyl-1,6-octadien-3-ol/ C_{10}H_{18}O</td>
<td>1.19 1.07</td>
<td></td>
<td>1236.010</td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>3,7-dimethyl-1,6-octadienal/ C_{10}H_{16}O</td>
<td>2.98 1.68</td>
<td></td>
<td>1239.191</td>
<td></td>
</tr>
<tr>
<td>37</td>
<td>4-(1-methylethyl)-1-Cyclohexene-1-carboxaldehyde/C_{10}H_{16}O</td>
<td>3.08</td>
<td></td>
<td>1237.223</td>
<td></td>
</tr>
<tr>
<td>38</td>
<td>4-(1-methylethyl)-1,5-Cyclohexadiene-1-methanol/C_{10}H_{16}O</td>
<td>0.06 0.10</td>
<td></td>
<td>1240.781</td>
<td></td>
</tr>
<tr>
<td>39</td>
<td>(E)-3,7-dimethyl-2,6-Octadien-1-ol/C_{10}H_{18}O</td>
<td>4.77</td>
<td></td>
<td>1241.188</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>1-methoxy-4-(1-propenyl)-Benzene/C_{10}H_{12}O</td>
<td>0.19</td>
<td></td>
<td>1251.485</td>
<td></td>
</tr>
<tr>
<td>41</td>
<td>Bornyl acetate/C_{12}H_{20}O_{2}</td>
<td></td>
<td>0.42</td>
<td>1254.937</td>
<td></td>
</tr>
<tr>
<td>42</td>
<td>acetate-1,7,7-trimethyl- Bicyclo[2.2.1]heptan-2-ol/C_{12}H_{20}O_{2}</td>
<td></td>
<td>0.74</td>
<td>1259.159</td>
<td></td>
</tr>
<tr>
<td>43</td>
<td>2-Dodecanone/C_{12}H_{24}O</td>
<td>0.84 0.64</td>
<td></td>
<td>1267.843</td>
<td></td>
</tr>
<tr>
<td>44</td>
<td>(-)-Myrtenyl acetate/C_{12}H_{18}O_{2}</td>
<td>0.03</td>
<td></td>
<td>1293.186</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>(3R-trans)-4-ethenyl-4-methyl-3-(1-methylethyl)-Bicyclo[2.2.1]heptan-2-ol/C_{12}H_{20}O_{2}</td>
<td>0.02</td>
<td></td>
<td>1319.098</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chemical Structure</td>
<td>Mass</td>
<td>Ions</td>
<td>Retention Time</td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>--------------------------------------------------------</td>
<td>--------</td>
<td>--------</td>
<td>----------------</td>
<td></td>
</tr>
<tr>
<td>48</td>
<td>(+)-Cycloisosativene/C$<em>{15}$H$</em>{24}$</td>
<td></td>
<td>0.10</td>
<td>0.11</td>
<td></td>
</tr>
<tr>
<td>49</td>
<td>(Z)-acetate-3,7-dimethyl-2,6-Octadien-1-ol/C$<em>{12}$H$</em>{20}$O$_{2}$</td>
<td></td>
<td>2.71</td>
<td>1.10</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>[1S-(1α.,2β,4β)]-1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-Cyclohexane/C$<em>{15}$H$</em>{24}$</td>
<td></td>
<td>0.20</td>
<td>0.19</td>
<td></td>
</tr>
<tr>
<td>51</td>
<td>γ-Elemene/C$<em>{15}$H$</em>{24}$</td>
<td></td>
<td>0.15</td>
<td>0.10</td>
<td></td>
</tr>
<tr>
<td>52</td>
<td>[1aR-(1αa.,4αa,7αa,7αb,7βa)]-decahydro-1,1,7-trimethyl-4-methylene-1H-Cycloprop[e]azulene/C$<em>{15}$H$</em>{24}$</td>
<td></td>
<td>0.19</td>
<td></td>
<td></td>
</tr>
<tr>
<td>53</td>
<td>(Z)-11-dimethyl-3-methylene-1,6,10-Dodecatriene/C$<em>{15}$H$</em>{24}$</td>
<td></td>
<td></td>
<td>0.11</td>
<td></td>
</tr>
<tr>
<td>54</td>
<td>1-(1,5-dimethyl-4-hexenyl)-4-methyl-Benzene/C$<em>{15}$H$</em>{22}$</td>
<td></td>
<td>0.53</td>
<td>3.19</td>
<td></td>
</tr>
<tr>
<td>55</td>
<td>α-Farnesene/C$<em>{15}$H$</em>{24}$</td>
<td></td>
<td>4.13</td>
<td>4.17</td>
<td></td>
</tr>
<tr>
<td>56</td>
<td>[s-(R@,s@)]-3-(1,5-dimethyl-4-hexenyl)-6-methylene-Cyclohexene/C$<em>{15}$H$</em>{24}$</td>
<td></td>
<td>4.09</td>
<td>4.33</td>
<td></td>
</tr>
<tr>
<td>57</td>
<td>[1R-(1α,3α,4β)]-4-ethenyl-α, α, 4-trimethyl-3-(1-methylethenyl)-Cyclohexanemethanol/C$<em>{15}$H$</em>{26}$O</td>
<td></td>
<td>0.46</td>
<td>0.29</td>
<td></td>
</tr>
<tr>
<td>No.</td>
<td>Compound</td>
<td>rc</td>
<td>RI</td>
<td>——</td>
<td>——</td>
</tr>
<tr>
<td>-----</td>
<td>-----------------------------------------------</td>
<td>-----</td>
<td>------</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>62</td>
<td>Heptadecane/C$<em>{17}$H$</em>{36}$</td>
<td>0.23</td>
<td>——</td>
<td>——</td>
<td>——</td>
</tr>
<tr>
<td>63</td>
<td>Tetradecanoic acid/C$<em>{14}$H$</em>{28}$O$_{2}$</td>
<td>1.33</td>
<td>——</td>
<td>——</td>
<td>——</td>
</tr>
<tr>
<td>64</td>
<td>6,10,14-trimethyl-2-Pentadecanone/C$<em>{18}$H$</em>{36}$O$_{1}$</td>
<td>1.45</td>
<td>——</td>
<td>0.09</td>
<td>——</td>
</tr>
<tr>
<td>65</td>
<td>(E,E)-6,10,14-trimethyl-5,9,13-Pentadecatrien-2-one/C$<em>{18}$H$</em>{30}$O$_{1}$</td>
<td>0.13</td>
<td>——</td>
<td>0.02</td>
<td>——</td>
</tr>
<tr>
<td>66</td>
<td>Dibutyl phthalate/C$<em>{16}$H$</em>{22}$O$_{4}$</td>
<td>——</td>
<td>——</td>
<td>——</td>
<td>0.04</td>
</tr>
<tr>
<td>67</td>
<td>n-Hexadecanoic acid/C$<em>{17}$H$</em>{34}$O$_{2}$</td>
<td>6.36</td>
<td>——</td>
<td>——</td>
<td>——</td>
</tr>
</tbody>
</table>

rc: Relative content (%); RI: Retention index; ——: not founded
Disclaimer

This article has been downloaded from WebmedCentral. With our unique author driven post publication peer review, contents posted on this web portal do not undergo any prepublication peer or editorial review. It is completely the responsibility of the authors to ensure not only scientific and ethical standards of the manuscript but also its grammatical accuracy. Authors must ensure that they obtain all the necessary permissions before submitting any information that requires obtaining a consent or approval from a third party. Authors should also ensure not to submit any information which they do not have the copyright of or of which they have transferred the copyrights to a third party.

Contents on WebmedCentral are purely for biomedical researchers and scientists. They are not meant to cater to the needs of an individual patient. The web portal or any content(s) therein is neither designed to support, nor replace, the relationship that exists between a patient/site visitor and his/her physician. Your use of the WebmedCentral site and its contents is entirely at your own risk. We do not take any responsibility for any harm that you may suffer or inflict on a third person by following the contents of this website.
Reviews

Review 1

Review Title: Analysis of common volatile constituents between herbal pair Ephedra sinica Stapf-Zingiber officinale Rosc and its single herb by GC-MS combined with AMWFA Method

Posted by Ms. Ai-lan Zhu on 12 Dec 2010 10:03:08 AM GMT

1. Is the subject of the article within the scope of the subject category? Yes
2. Are the interpretations / conclusions sound and justified by the data? Yes
3. Is this a new and original contribution? Yes
4. Does this paper exemplify an awareness of other research on the topic? Yes
5. Are structure and length satisfactory? Yes
6. Can you suggest brief additions or amendments or an introductory statement that will increase the value of this paper for an international audience? No
7. Can you suggest any reductions in the paper, or deletions of parts? No
8. Is the quality of the diction satisfactory? Yes
9. Are the illustrations and tables necessary and acceptable? Yes
10. Are the references adequate and are they all necessary? Yes
11. Are the keywords and abstract or summary informative? Yes

Rating: 7

Comment:
The authors analyzed the common volatile constituents between herbal pair (HP) Ephedra sinica Stapf?ESS? -Zingiber officinal Rosc ?ZOR?and its single herb by the method of GC-MS and alternative moving window factor analysis (AMWFA). Many researchers who are interested in Chinese Medicine will benefit from this paper.

Competing interests: none

Invited by the author to make a review on this article? : Yes

Experience and credentials in the specific area of science: yes

Publications in the same or a related area of science: No

How to cite: Zhu A. Analysis of common volatile constituents between herbal pair Ephedra sinica Stapf-Zingiber officinale Rosc and its single herb by GC-MS combined with AMWFA Method|Review of the article 'Analysis Of Common Volatile Constituents Between Herbal Pair Ephedra Sinica Stapf-Zingiber Officinale Rosc And Its Single Herb By Gc-ms Combined With Amwfa Method' by |WebmedCentral 1970;1(12):REVIEW_REF_NUM233
Review 2

Review Title: Analysis of common volatile constituents between herbal pair Ephedra sinica Stapf-Zingiber officinale Rosc and its single herb by GC-MS combined with AMWFA Method

Posted by Mr. Wei Daijin on 12 Dec 2010 06:07:08 AM GMT

1. Is the subject of the article within the scope of the subject category? Yes
2. Are the interpretations / conclusions sound and justified by the data? Yes
3. Is this a new and original contribution? Yes
4. Does this paper exemplify an awareness of other research on the topic? Yes
5. Are structure and length satisfactory? Yes
6. Can you suggest brief additions or amendments or an introductory statement that will increase the value of this paper for an international audience? No
7. Can you suggest any reductions in the paper, or deletions of parts? No
8. Is the quality of the diction satisfactory? Yes
9. Are the illustrations and tables necessary and acceptable? Yes
10. Are the references adequate and are they all necessary? Yes
11. Are the keywords and abstract or summary informative? Yes

Rating: 7

Comment:
This article is suitable for publication. The strength of the chemometric techniques assisted with PTRIs in obtaining more information from the GC–MS data is demonstrated in this investigation.

Competing interests: none

Invited by the author to make a review on this article?: Yes

Experience and credentials in the specific area of science: yes

Publications in the same or a related area of science: No

Review 3

Review Title: Analysis of common volatile constituents between herbal pair Ephedra sinica Stapf-Zingiber officinale Rosc and its single herb by GC-MS combined with AMWFA Method

Posted by Prof. Yue-Long Liu on 12 Dec 2010 03:01:38 AM GMT

1. Is the subject of the article within the scope of the subject category? Yes
2. Are the interpretations / conclusions sound and justified by the data? Yes
3. Is this a new and original contribution? Yes
4. Does this paper exemplify an awareness of other research on the topic? Yes
5. Are structure and length satisfactory? Yes
6. Can you suggest brief additions or amendments or an introductory statement that will increase the value of this paper for an international audience? No
7. Can you suggest any reductions in the paper, or deletions of parts? No
8. Is the quality of the diction satisfactory? Yes
9. Are the illustrations and tables necessary and acceptable? Yes
10. Are the references adequate and are they all necessary? Yes
11. Are the keywords and abstract or summary informative? Yes

Rating: 8

Comment:
In this paper, the essential oils of the herb pair and two single herbs ESS and ZOR have been investigated for the first time. The information about the chemical constituents of essential oils is useful and necessary to the further pharmacological study of the recipe ESS-ZOR, which will certainly help us to utilize the recipe ESS-ZOR better.

Competing interests: none

Invited by the author to make a review on this article? Yes

Experience and credentials in the specific area of science: Yes

Publications in the same or a related area of science: No

How to cite: Liu Y. Analysis of common volatile constituents between herbal pair Ephedra sinica Stapf-Zingiber officinale Rosc and its single herb by GC-MS combined with AMWFA Method[Review of the article 'Analysis Of Common Volatile Constituents Between Herbal Pair Ephedra Sinica Stapf-zingiber Officinale Rosc And Its Single Herb By Gc-ms Combined With Amwfa Method ' by ].WebmedCentral 1970;1(12):REVIEW_REF_NUM231
Review 4

Review Title: Analysis of common volatile constituents between herbal pair Ephedra sinica Stapf-Zingiber officinale Rosc and its single herb by GC-MS combined with AMWFA Method

Posted by Ms. Shuai-Hua Chen on 11 Dec 2010 03:09:11 PM GMT

| 1 | Is the subject of the article within the scope of the subject category? | Yes |
| 2 | Are the interpretations / conclusions sound and justified by the data? | Yes |
| 3 | Is this a new and original contribution? | Yes |
| 4 | Does this paper exemplify an awareness of other research on the topic? | Yes |
| 5 | Are structure and length satisfactory? | Yes |
| 6 | Can you suggest brief additions or amendments or an introductory statement that will increase the value of this paper for an international audience? | No |
| 7 | Can you suggest any reductions in the paper, or deletions of parts? | No |
| 8 | Is the quality of the diction satisfactory? | Yes |
| 9 | Are the illustrations and tables necessary and acceptable? | Yes |
| 10 | Are the references adequate and are they all necessary? | Yes |
| 11 | Are the keywords and abstract or summary informative? | Yes |

Rating: 8

Comment:
This article is suitable for publication. Many researchers will be interested in it. The aim of this research work is at systematically investigating of the volatile chemical components of ESS, ZOR, and the HP by the method of gas chromatography—mass spectrometry (GC-MS) and alternative moving window factor analysis (AMWFA).

Competing interests: none

Invited by the author to make a review on this article? : Yes

Experience and credentials in the specific area of science: yes

Publications in the same or a related area of science: No

How to cite: Chen S. Analysis of common volatile constituents between herbal pair Ephedra sinica Stapf-Zingiber officinale Rosc and its single herb by GC-MS combined with AMWFA Method[Review of the article 'Analysis Of Common Volatile Constituents Between Herbal Pair Ephedra Sinica Stapf-zingiber Officinale Rosc And Its Single Herb By Gc-ms Combined With Amwfa Method ' by ],WebmedCentral 1970;1(12):REVIEW_REF_NUM228
Disclaimer

This article has been downloaded from WebmedCentral. With our unique author driven post publication peer review, contents posted on this web portal do not undergo any prepublication peer or editorial review. It is completely the responsibility of the authors to ensure not only scientific and ethical standards of the manuscript but also its grammatical accuracy. Authors must ensure that they obtain all the necessary permissions before submitting any information that requires obtaining a consent or approval from a third party. Authors should also ensure not to submit any information which they do not have the copyright of or of which they have transferred the copyrights to a third party.

Contents on WebmedCentral are purely for biomedical researchers and scientists. They are not meant to cater to the needs of an individual patient. The web portal or any content(s) therein is neither designed to support, nor replace, the relationship that exists between a patient/site visitor and his/her physician. Your use of the WebmedCentral site and its contents is entirely at your own risk. We do not take any responsibility for any harm that you may suffer or inflict on a third person by following the contents of this website.