COMPOSITION OF ESSENTIAL OIL ISOLATED FROM MARIGOLD (TAGETES ERECTA L.) FLOWERS CULTIVATED IN LAHORE, PAKISTAN

MALIK FIAZ HUSSAIN FERDOSI*, IQRA HAIDER KHAN† AND ARSHAD JAVAID†

Department of Horticulture, Faculty of Agricultural Sciences, University of the Punjab, Quaid-i-Azam Campus, Lahore 54590, Pakistan

Keywords: Essential oil, GC-MS, Marigold, Pakistan

Abstract

The composition of essential oil of marigold (Tagetes erecta L.) flowers was investigated. The oil was analyzed by GC-MS for identification of various components. Among these, 3-cyclohexene-1-methanol, α, α,4-trimethyl-, acetate was the most abundant compound (31.67%) followed by phenol, 2,4-bis (1,1-dimethylethyl)- (14.35%) and eucalyptol (14.27%). Other compounds included dodecanoic acid (5.97%), tetradecanoic acid (5.58%), octadecane (4.93%), propanoic acid, 2-bromo-2-methyl-, ethyl ester (5.43%), cyclohexanol, 1-methyl-4-(1-methylethanyl)-, acetate (5.33), n-hexadecanoic acid (4.70), p-menth-1-en-8-ol (4.20%) and thymol (3.57%).

Introduction

Tagetes erecta L. belonging to Asteraceae, is native to Mexico and has medicinal, pharmaceutical, aromatic and ornamental properties (Abbas et al. 2019). It is an annual drought resistant plant grown widely because of its beautiful flowers and easy availability throughout the year. It is a commercially exploited floriculture crop of Pakistan planted in bedding of landscape areas (Zulfiqar et al. 2020). Plant possesses large size cut flowers, which are different in shape, color and size. The flowers are sold in the market as loose flowers and highly suitable for beautification (Aslam et al. 2016). It is used as a flavoring agent and an edible dye as a substitute of saffron, which yields the yellow color (Sowndharya and Giri 2020). It has antioxidant, nematicidal and phenolic compounds, which are used in the preparation of medicines (Ayub et al. 2017).

Essential oils (EOs) play a vital role in plants by producing a specific aroma, flavor and to protect the plant from pathogens (Perczak et al. 2019). These characteristics, together with their diverse biological activities have attracted high interest from medicine, perfumery and food processing industry (Ayaz et al. 2017). T. erecta flowers are a rich source of secondary metabolites such as carotenoids, lutein, triterpenes, thiophenes and flavonoids (Kazibwe et al. 2017). Essential oil prepared from T. erecta flowers possesses complex composition of aromatic and volatile components which exhibited a wide range of anti-inflammatory, antinociceptive, antioxidant, insecticidal, antifungal, anticancer, antiepileptic, allelopathic, larvicidal, hepatoprotective, anti-diabetic, antidepressant, wound healing and mosquitocidal activities (Safar et al. 2020). Therefore, the present study was undertaken to assess the composition of essential oil of marigold flowers cultivated in Pakistan.

Materials and Methods

The present research work was carried out at the Faculty of Agricultural Sciences, University of the Punjab, Lahore, Pakistan; and Pakistan Council of Scientific and Industrial Research (PCSIR) Laboratories, Lahore, Pakistan. Full bloomed, healthy looking fresh flowers of marigold

*Author for correspondence: <malikferdosi@yahoo.com>, <fiaz.iags@pu.edu.pk>. †Department of Plant Pathology, Faculty of Agricultural Sciences, University of the Punjab, Quaid-i-Azam Campus, Lahore 54590, Pakistan.
were plucked from Punjab University Lahore. Plucking of flowers was done early in the morning to avoid any possible loss of essential oil. Paper boxes were used to transfer flowers into the laboratory for further study process. Only the flower petals were used for the recovery of essential oil. Methanol was used as organic solvent in the Soxhlet’s extraction apparatus. Volatile oil was sucked up by siphon in the thimble along with methanol through the condensers. The process was repeated 3-4 times. After taking out whole aroma out from the flowers, rotary evaporator was used for the distillation of recovered solvent.

The oil was analyzed for its chemical components. Gas chromatography 6890 Agilent /mass spectroscopy 5973 Agilent were used for identification of various constituents of essential oil. To obtain the chemical composition, sample of the extracted oil was injected with a syringe into the GC and was run as per set conditions: oven initial temperature was 50 ºC, column DB-5 (30 m × 0.3 µm × 0.25 µm), ramping: 7 ºC/min till 230 ºC, final temperature was 230 ºC for 5 min. Injector temperature was 180 ºC, carrier gas was helium, flow rate 1.0 µl/min, split less, volume 0.3 µl, µS: source temperature 230 ºC, Quad 150, 70 ev, EI. MS was done by comparing the chromatogram with library.

Results and Discussion

GC-MS chromatogram indicated that there were 11 constituents in essential oil of marigold (Fig. 1). Details of these compounds regarding their retention times, peak area percentages, molecular formulae and molecular weights are presented in Table 1. Among these, 3-cyclohexene-1-methanol, α, α,4-trimethyl-, acetate (31.67%), also known as α-terpinyl acetate, was the principal constituent of the essential oil of marigold. In contrast to the present study, Gutterrez et al. (2006) reported piperetone (19.2%) followed by β-caryophyllene (15.2%) as the major components of essential oil in flowers of marigold collected from Mexico. Likewise, Krishna et al. (2004) also found piperetone (28.5%) followed by piperitenone (10.9%) as the major components of essential oil of marigold flower collected from India. On the other hand, Iranian marigold contained β-caryophyllene (35.2%) as major component of essential oil of flower (Sefidkon et al. 2004). Similar differences in chemical compositions have also been reported in essential oils of other plants such as Artemisia lavandulaefolia (Zhang et al. 2012). The differences in chemical composition of essential oil of the same species could be attributed to seasonal and geographic factors (Huang et al. 2018). α-terpinyl acetate, a natural monoterpene ester and a commercially

![Fig. 1. GC-MS chromatogram of essential oil of marigold.](image-url)
significant fragrance molecule. has also been reported as a major constituent of essential oils of *Stachys setifera* ssp. *iranica* (11.2%), *Chamaecyparis obtusa* (13.71%) and *Elettaria cardamomum* (46.12%) (Javidnia et al. 2003, Yang et al. 2007, Chowdhury and Kumar 2020). This compound possesses antioxidant and anti-amyloidogenic properties and also has disease amelioration effects in Alzheimer's disease (Chowdhury and Kumar 2020).

Table 1. Compounds identified in essential oil of marigold flowers by GC-MS analysis.

<table>
<thead>
<tr>
<th>Sl. No.</th>
<th>Names of compounds</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
<th>Retention time (min)</th>
<th>Peak area (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Propanoic acid, 2-bromo-2-methyl-, ethyl ester</td>
<td>C_{10}H_{16}O</td>
<td>195.05</td>
<td>5.116</td>
<td>5.43</td>
</tr>
<tr>
<td>2</td>
<td>Cyclohexanol, 1-methyl-4-(1-methylethanyl)-, acetate</td>
<td>C_{12}H_{30}O_{2}</td>
<td>196.28</td>
<td>5.693</td>
<td>5.33</td>
</tr>
<tr>
<td>3</td>
<td>Eucalyptol</td>
<td>C_{10}H_{18}O</td>
<td>154.25</td>
<td>5.943</td>
<td>14.27</td>
</tr>
<tr>
<td>4</td>
<td>p-Menth-1-en-8-ol</td>
<td>C_{10}H_{18}O</td>
<td>154.25</td>
<td>8.862</td>
<td>4.20</td>
</tr>
<tr>
<td>5</td>
<td>3-Cyclohexene-1-methanol, α, α,4-trimethyl-, acetate</td>
<td>C_{12}H_{30}O_{2}</td>
<td>196.29</td>
<td>10.844</td>
<td>31.67</td>
</tr>
<tr>
<td>6</td>
<td>Thymol</td>
<td>C_{10}H_{14}O</td>
<td>150.22</td>
<td>12.617</td>
<td>3.57</td>
</tr>
<tr>
<td>7</td>
<td>Phenol, 2,4-bis(1,1-dimethylethyl)-</td>
<td>C_{14}H_{20}O</td>
<td>206.32</td>
<td>13.058</td>
<td>14.35</td>
</tr>
<tr>
<td>8</td>
<td>Dodecanoic acid</td>
<td>C_{12}H_{22}O_{2}</td>
<td>200.32</td>
<td>13.396</td>
<td>5.97</td>
</tr>
<tr>
<td>9</td>
<td>Octadecane</td>
<td>C_{18}H_{36}</td>
<td>254.5</td>
<td>14.917</td>
<td>4.93</td>
</tr>
<tr>
<td>10</td>
<td>Tetradecanoic acid</td>
<td>C_{14}H_{29}O_{2}</td>
<td>228.37</td>
<td>15.626</td>
<td>5.58</td>
</tr>
<tr>
<td>11</td>
<td>n-Hexadecanoic acid</td>
<td>C_{16}H_{32}O_{2}</td>
<td>256.42</td>
<td>17.684</td>
<td>4.70</td>
</tr>
</tbody>
</table>

Two compounds, namely phenol 2,4-bis (1,1-dimethylethyl)- (14.35%) and eucalyptol (14.27%) were found as abundantly occurring components of essential oil in the present study (Table 1). Phenol, 2,4-bis (1,1-dimethylethyl)- or 2,4-di-tert-butylphenol is a familiar secondary metabolite produced by a variety of organisms including bacteria, fungi, liverworts, diatom, plants and animals. It has antioxidant, anti-inflammatory, cytotoxic, insecticidal, antibacterial, antiviral, antifungal, phytoxic and nematicidal activities (Zhao et al. 2020). Eucalyptol or 1,8-cineole, a monoterpenoid, a colorless liquid, having mint-like smell and made up 90% of eucalyptus oil (Boland et al. 1991), was found as a major constituent in essential oils of a variety of plant species including *Helichrysum gymnocephalum* (47.4%), *Rosmarinus officinalis* (43.7%) and *Artemisia lavandulafolia* (35.60%) (Afoulous et al. 2011, Rašković et al. 2014, Huang et al. 2018). This compound has a number of biological activities including antibacterial, anti-inflammatory, antihypertensive and percutaneous penetration enhancer (Jiang et al. 2019). It has also been used in cosmetics, fragrances and as a flavoring agent (Bhowal and Gopal 2015).

Compounds present in moderate concentrations in essential oil of marigold included dodecanoic acid (5.97%), tetradecanoic acid (5.58%), octadecane (4.93%), propanoic acid, 2-bromo-2-methyl-, ethyl ester (5.43%), cyclohexanol, 1-methyl-4-(1-methylethanyl)-, acetate (5.33), n-hexadecanoic acid (4.70), p-menth-1-en-8-ol (4.20%) and thymol (3.57%) (Table 1). Dodecanoic acid or lauric acid, medium-chain white powdery solid saturated fatty acid and a major component of coconut oil (45-53%) possessed strong antibacterial, antifungal and antiviral potential (Dayrit 2014). Tetradecanoic acid or myristic acid is a long-chain saturated fatty acid...
Table 2. Properties of compounds identified in essential oil of marigold flowers by GC-MS analysis.

<table>
<thead>
<tr>
<th>Sl. No.</th>
<th>Names of compounds</th>
<th>Bioactivity</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Propanoic acid, 2-bromo-2-methyl-, ethyl ester</td>
<td>Not reported</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>Cyclohexanol, 1-methyl-4-(1-methylene)-, acetate</td>
<td>Not reported</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>Eucalyptol</td>
<td>Anti-inflammatory, antinociceptive, antihypertensive, antibacterial</td>
<td>Santos and Rao (2000),</td>
</tr>
<tr>
<td>4</td>
<td>p-Menth-1-en-8-ol</td>
<td>Antioxidant, anti-proliferative, anti-inflammatory, antimicrobial</td>
<td>Sales et al. (2020)</td>
</tr>
<tr>
<td>5</td>
<td>3-Cyclohexene-1-methanol, α, α,4-trimethyl-, acetate</td>
<td>Antioxidant, anti-amyloidogenic</td>
<td>Chowdhury and Kumar (2020)</td>
</tr>
<tr>
<td>6</td>
<td>Thymol</td>
<td>Antifungal, antibacterial, free radical scavenging, analgesic, anti-inflammatory, antioxidant, antispasmodic, antiseptic, antitumor</td>
<td>Meenan et al. (2017)</td>
</tr>
<tr>
<td>7</td>
<td>Phenol, 2,4-bis(1,1-dimethylene)-</td>
<td>Antioxidant, anti-inflammatory, cytotoxic, insecticidal, antibacterial, antiviral, antifungal, phytotoxic and nematicidal</td>
<td>Zhao et al. (2020)</td>
</tr>
<tr>
<td>8</td>
<td>Dodecanoic acid</td>
<td>Antimicrobial, antifungal and antiviral</td>
<td>Dayrit (2014)</td>
</tr>
<tr>
<td>9</td>
<td>Octadecane</td>
<td>Antibacterial, antifungal</td>
<td>Jasim et al. (2015), Barupal et al. (2019)</td>
</tr>
<tr>
<td>10</td>
<td>Tetradecanoic acid</td>
<td>Antifungal, antioxidant, nematicide</td>
<td>Mujeeb et al. (2014)</td>
</tr>
</tbody>
</table>

mostly found in milk and had antifungal, antioxidant, nematicide properties (Mujeeb et al. 2014). n-Hexadecanoic acid or palmitic acid is the most widespread saturated fatty acid in plants, animals as well as in microorganisms (Ferdosi et al. 2021, Javaid et al. 2021, Khan et al. 2021). It exhibited considerable cytotoxicity against human colorectal carcinoma cells (Ravi and Krishman 2017). p-Menth-1-en-8-ol or α-terpineol, a monoterpenoid alcohol, was known for its multiple biological properties such as antioxidant, anticarcinogenic anti-inflammatory, antimicrobial and anticonvulsant (Sales et al. 2020). Thymol, a monoterpenic phenol, possessed a variety of pharmacological properties such as antifungal, antibacterial, free radical scavenging, analgesic, anti-inflammatory, antioxidant, antispasmodic, antiseptic and antitumor activities (Meenan et al. 2017). From the present study it may be concluded that essential oil of marigold flowers from Pakistan contains a variety of bioactive substance.
COMPOSITION OF ESSENTIAL OIL ISOLATED FROM MARIGOLD

References


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