CHAPTER 2

ESSENTIAL OIL COMPOSITION OF BURDELLA ASIATICA AND ITS COMPARISON WITH ITS ALLIED SPECIES
Buddleja asiatica

Buddleja davidii
Estelar
2.1 PLANT MATERIAL

The fresh aerial parts of *Buddleja asiatica* Lour. were collected from Jeolikote, Nainital in the month of February, 2009. The plant identification was confirmed by the Botanical Survey of India (BSI), Dehradun. A voucher specimen (No.112965) was deposited in the Herbarium Section at BSI, Dehradun, India.

2.2 EXPERIMENTAL

2.2.1 Essential Oil Extraction

The fresh aerial parts (5 kg) were chopped and steam-distilled using copper still fitted with spiral glass condensers. The distillate was saturated with NaCl and extracted with *n*-hexane. Anhydrous Na$_2$SO$_4$ was then added to dry the organic phase which was separated using separating funnel and finally the solvent was evaporated under reduced pressure. The percentage content was calculated on the basis of dry weight of plant material. The oil was then stored in screw-capped vials, under refrigeration until needed.
2.2.2 GC-MS Analysis

The oil was analysed on Nucon 5765 GC (30mx0.32mm, FID) with split ratio 1:48, N₂ flow of 4.0 kg/cm². GC/MS was done on thermoquest trace GC-2000 interfaced with Finnigen MAT Polaries-Q ion trap mass spectrometer fitted with RTX-5MS (Restek Corporation) fused silica capillary column (30 x 0.25 mm, 0.25 μm film coating). The oven temperature was programmed from 60-210°C at 3°C/min using Helium as carrier gas at 1.0 ml/min. The injector temperature was 210°C, injection volume was 0.1µl prepared in hexane, split ratio 1:40. Mass spectra were taken at 70ev (EI) with mass scan range of m/z 40-450 amu with mass scan time 4 seconds.

2.3 RESULTS AND DISCUSSION

The steam distillation of aerial parts of *B. asiatica* (B1) yielded 0.01% (w/w) of the essential oil. The oil sample was analysed by GC and GC-MS and the identification of the essential oil components was accomplished by comparison of their GC-MS retention indices as well as their mass spectra with corresponding data of authentic components of reference oils by using library mass search database (NIST &WILEY) and Robert P. Adams (Adams, 1995). To minimize the standard deviation
arising from employing a sole substance as internal standard, it was decided to employ a retention index, namely, Kovat’s Index obtained by using a homologous series of \( n \)-alkanes C9-C22. This approach greatly improved the identification, especially for those compounds with very similar fragmentation patterns. The gas chromatogram of \( B. asiatica \) is shown in Fig. 1. A total of 15 constituents were identified representing 83.69% of the total oil. The major constituents were \( n \)-tridecane (55.87%), 5-methylundecane (10.62%), \( n \)-dodecane (2.84%), \( n \)-hexadecanol (2.76%). The results clearly indicate that the essential oil contains many aliphatic hydrocarbons.

The literature survey revealed that the essential oil from \( Buddleja asiatica \) reported by Garg and Dengre (1992) appeared to be completely different from the present study. These variations indicated that the dynamics of essential composition in aromatic plants is possibly associated with the climatic and regional variations (Atti-Santos et al., 2004; Muller-Riebau et al., 1997; Aziz et al., 2010). It was considered that further investigation should be carried out to define the chemotype of \( B. asiatica \).
Fig. 1
2.3.1 Essential oil composition of allied species of *B. asiatica*

*Buddleja davidii* belonging to family Buddlejaceae, is a native of Sichuan and Hubei provinces in central China and of Japan. The plant is a vigorous shrub with an arching habit and is widely used as an ornamental plant (Phillips and Rix, 1994). The fresh aerial parts of *B. davidii* (5kg) were collected from Nainital in the month of September, 2009. The plant identification was confirmed by Himalayan Botanical Garden (HBG), Nainital, Uttarakhand, India. A voucher specimen (No.865) was deposited in the Herbarium Section at HBG, Nainital, India.

Essential oil extraction from aerial parts of the plant and GC, GC-MS analysis were done by the same procedure as described earlier.

The steam distillation of aerial parts of *Buddleja davidii* (B2) yielded 0.03% (w/w) of the essential oil. The identification of essential oil components was done on the basis of retention index, library mass search database (NIST &WILEY) and Robert P. Adams (Adams, 1995). The gas chromatogram of *B. davidii* is shown in Fig. 2. A total of 17 constituents were identified representing 86.83% of the total oil. The major constituents were *n*-dodecane (55.15%), 5- methylundecane (13.67%), *iso*-acorone (4.32%), *n*-undecane (2.64%).
A comparative study of the essential oil composition of *B. asiatica* and *B. davidii* aerial parts is presented in Table 4. Interestingly the major component detected in *B. asiatica* essential oil was found as minor component in *B. davidii* essential oil and vice-versa. Furthermore among the major constituents identified in *B. davidii* essential oil, iso-acorone was found absent in *B. asiatica* oil while 5-methylundecane was present as one of the major components in both the oils.

The available literature indicates lack of work published on the chemical composition of *B. davidii* essential oil, therefore, the present study was carried out to investigate the essential oil composition of *B. davidii* aerial parts and its comparison with that of *B. asiatica* aerial parts essential oil.
Fig. 2
Table 4: Essential oil composition of *B. asiatica* (B1) and *B. davidii* (B2) aerial parts

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Compounds</th>
<th>KI</th>
<th>Oil %</th>
<th>Mode of Identification</th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>B1</td>
<td>B2</td>
</tr>
<tr>
<td>1</td>
<td>2,2,5-trimethyl-3,4-hexanedione</td>
<td>800</td>
<td>0.96</td>
<td>-</td>
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<tr>
<td>2</td>
<td>4-propyl-6-heptadien-4-ol</td>
<td>880</td>
<td>1.17</td>
<td>-</td>
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<tr>
<td>3</td>
<td><em>n</em>-undecane</td>
<td>1110</td>
<td>1.50</td>
<td>2.64</td>
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<tr>
<td>4</td>
<td>Terpineol &lt;cis-β&gt;</td>
<td>1140</td>
<td>0.23</td>
<td>1.02</td>
</tr>
<tr>
<td>5</td>
<td>5-methylundecane</td>
<td>1160</td>
<td>10.62</td>
<td>13.67</td>
</tr>
<tr>
<td>6</td>
<td>4-methylundecane</td>
<td>1170</td>
<td>0.86</td>
<td>0.40</td>
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<tr>
<td>7</td>
<td><em>n</em>-dodecane</td>
<td>1205</td>
<td>2.84</td>
<td>55.15</td>
</tr>
<tr>
<td>8</td>
<td>6-methyldodecane</td>
<td>1220</td>
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<td>2.38</td>
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<tr>
<td>9</td>
<td><em>n</em>-tridecane</td>
<td>1300</td>
<td>55.87</td>
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</tr>
<tr>
<td>10</td>
<td>2,3-dimethylnonane</td>
<td>1340</td>
<td>-</td>
<td>0.50</td>
</tr>
<tr>
<td>11</td>
<td><em>Bis</em>(1,1-dimethylethyl)diazene</td>
<td>1350</td>
<td>0.83</td>
<td>-</td>
</tr>
<tr>
<td>12</td>
<td>3-methyltridecane</td>
<td>1355</td>
<td>0.39</td>
<td>0.54</td>
</tr>
<tr>
<td>13</td>
<td><em>n</em>-tetradecane</td>
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<td>0.66</td>
<td>0.71</td>
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<td>14</td>
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<td>1.79</td>
<td>0.40</td>
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<tr>
<td>15</td>
<td>&lt;iso-&gt; acorone</td>
<td>1815</td>
<td>-</td>
<td>4.32</td>
</tr>
<tr>
<td>16</td>
<td><em>n</em>-hexadecanol</td>
<td>1865</td>
<td>2.76</td>
<td>0.77</td>
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<tr>
<td>17</td>
<td>Cyclohexadecanolide</td>
<td>1930</td>
<td>-</td>
<td>0.61</td>
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<tr>
<td>18</td>
<td><em>n</em>-eicosane</td>
<td>1990</td>
<td>0.86</td>
<td>0.93</td>
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<tr>
<td>19</td>
<td><em>n</em>-octadecanol</td>
<td>2065</td>
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<tr>
<td>20</td>
<td><em>Trans-</em> totarol</td>
<td>2300</td>
<td>-</td>
<td>0.63</td>
</tr>
<tr>
<td></td>
<td><strong>Total</strong></td>
<td></td>
<td><strong>83.69</strong></td>
<td><strong>86.83</strong></td>
</tr>
</tbody>
</table>

a= mass spectra, b= KI

B1= *B. asiatica*, B2= *B. davidii*
2.4 REFERENCES


