



J. Serb. Chem. Soc. 76 (4) S1–S3 (2011)

SUPPLEMENTARY MATERIAL TO  
**Chemical investigation of the essential oil of *Laggera crispata*  
(Vahl) Hepper & Wood from India**

RAM S. VERMA<sup>1\*</sup>, RAJENDRA C. PADALIA<sup>1</sup>, CHANDAN S. CHANOTIYA<sup>2</sup>,  
AMIT CHAUHAN<sup>1</sup> and ANJU YADAV<sup>2</sup>

<sup>1</sup>Central Institute of Medicinal and Aromatic Plants (CIMAP, CSIR), Research Centre,  
Pantnagar, P. O. – Dairy farm Nagla, Udham Singh Nagar, Uttarakhand-263149  
and <sup>2</sup>Central Institute of Medicinal and Aromatic Plants (CIMAP, CSIR),  
P. O. CIMAP, Lucknow-226015, India

J. Serb. Chem. Soc. 76 (4) (2011) 523–528

TABLE I-S. Essential oil composition of *L. crispata* from the Kumaon region of Uttarakhand, India

Compound	Class	$R_I^a$	$R_I^b$	$R_I^c$	Peak area <sup>d</sup> , %
$\alpha$ -Thujene	MH	932	931	1028	tr
$\alpha$ -Pinene	MH	941	939	1022	tr
Sabinene	MH	978	976	1124	0.2
$\beta$ -Pinene	MH	982	980	1109	tr
$\beta$ -Myrcene	MH	989	991	1164	0.1
(Z)-3-Hexenyl acetate	AC	998	1004	–	tr
$\alpha$ -Phellandrene	MH	1000	1005	1167	0.5
$\delta$ -3-Carene	MH	1007	1011	1153	tr
$\alpha$ -Terpinene	MH	1012	1018	1179	0.3
<i>p</i> -Cymene	BC	1019	1026	1274	0.4
Limonene	MH	1024	1031	1198	0.1
$\beta$ -Phellandrene	MH	1029	1031	1210	tr
(Z)- $\beta$ -Ocimene	MH	1042	1040	1242	tr
(E)- $\beta$ -Ocimene	MH	1055	1050	1265	0.5
$\gamma$ -Terpinene	MH	1066	1062	1248	0.4
Terpinolene	MH	1087	1088	1284	0.1
(E)-Sabinene hydrate <sup>e</sup>	OM	1100	1097	1559	0.8
Linalool	OM	1103	1098	1555	tr
(Z)- <i>p</i> -Menth-2 en-1-ol	OM	1120	1121	1636	0.1
(E)- <i>p</i> -Menth-2 en-1-ol	OM	1137	1140	1570	0.1
(E)-Pinocamphone	OM	1157	1160	–	tr
Terpinen-4-ol	OM	1172	1177	1611	1.5
<i>p</i> -Cymen-8-ol	BC	1184	1183	1865	0.1

\* Corresponding author. E-mail: rswaroop1979@yahoo.com

TABLE I-S. Continued

Compound	Class	<i>R</i> <sub>f</sub> <sup>a</sup>	<i>R</i> <sub>f</sub> <sup>b</sup>	<i>R</i> <sub>f</sub> <sup>c</sup>	Peak area <sup>d</sup> , %
$\alpha$ -Terpineol	OM	1187	1189	1705	tr
Myrtenol	OM	1188	1194	1887	tr
Thymol methyl ether	BC	1234	1235	1597	0.1
Carvacrol methyl ether	BC	1245	1244	1618	0.1
Thymol	BC	1293	1290	–	tr
$\beta$ -Caryophyllene	SH	1426	1418	1589	6.9
2,5-Dimethoxy- <i>p</i> -cymene <sup>f</sup>	BC	1431	1423	1877	32.2
Aromadendrene	SH	1440	1439	–	tr
( <i>Z</i> )- $\beta$ -Farnesene	SH	1445	1443	1666	0.1
$\alpha$ -Humulene	SH	1456	1454	1685	2.0
( <i>E</i> )- $\beta$ -Farnesene	SH	1460	1458	1673	tr
$\beta$ -Acoradiene	SH	1466	1466	–	tr
$\gamma$ -Gurjunene	SH	1474	1473	–	tr
$\gamma$ -Muurolene	SH	1478	1477	–	tr
Germacrene D	SH	1481	1480	1728	tr
2-Phenylethyl propionate	BC	1483	–	–	0.9
$\beta$ -Selinene	SH	1486	1485	1713	0.1
$\alpha$ -Selinene	SH	1491	1494	1742	0.1
Bicyclogermacrene	SH	1496	1495	1754	1.8
$\alpha$ -Muurolene	SH	1500	1499	1737	tr
Germacrene A	SH	1502	1503	–	tr
$\beta$ -Bisabolene	SH	1508	1509	1743	tr
$\gamma$ -Cadinene	SH	1512	1513	–	tr
Cubebol	OS	1516	1514	1954	0.1
$\delta$ -Cadinene	SH	1527	1524	1771	0.1
( <i>Z</i> )-Nerolidol	OS	1533	1534	–	0.1
$\alpha$ -Cadinene	SH	1537	1538	1813	tr
$\alpha$ -Calacorene	SH	1542	1542	1937	0.3
Elemol	OS	1545	1549	2092	1.1
Thymohydroquinone	BC	1549	1553	–	tr
Germacrene B	SH	1559	1556	1854	tr
( <i>E</i> )-Nerolidol	OS	1563	1564	2048	tr
Germacrene D-4-ol	OS	1572	1574	2068	0.1
Caryophyllene oxide	OS	1583	1581	2005	5.4
Guaïol	OS	1596	1595	2100	0.1
Humulene epoxide II	OS	1607	1606	–	0.3
1,10- <i>di-epi</i> -Cubenol	OS	1611	1612	–	tr
10- <i>epi</i> - $\gamma$ Eudesmol	OS	1621	1619	2112	14.7
1- <i>epi</i> -Cubenol	OS	1627	1627	2085	0.3
$\gamma$ Eudesmol	OS	1629	1630	2184	0.6
<i>epi</i> - $\alpha$ -Cadinol	OS	1637	1640	–	0.4
<i>epi</i> - $\alpha$ -Muurolol	OS	1641	1641	2206	1.4
$\beta$ -Eudesmol	OS	1647	1649	2253	0.5
$\alpha$ -Eudesmol	OS	1651	1652	2247	0.9
7- <i>epi</i> - $\alpha$ -Eudesmol	OS	1656	1658	–	2.4
Bulnesol	OS	1667	1666	–	0.2

TABLE I-S. Continued

Compound	Class	$RI^a$	$RI^b$	$RI^c$	Peak area <sup>d</sup> , %
$\beta$ -Bisabolol	OS	1672	1671	2166	0.2
Eudesma-4(15),7-dien-1- $\beta$ -ol	OS	1684	1685	–	tr
Juniper camphor	OS	1692	1691	2319	3.4
( <i>Z,Z</i> )-Farnesol	OS	1715	1713	–	tr
Curcuphenol	BC	1717	1715	–	tr
( <i>E,E</i> )-Farnesol	OS	1721	1722	2366	tr
Oplopanone	OS	1735	1733	–	0.2
( <i>E,Z</i> )-Farnesol	OS	1745	1742	–	tr
Benzyl benzoate	BC	1762	1762	–	0.1
8- $\alpha$ -Acetoxyelemol <sup>g</sup>	OS	1790	1789	–	1.4
<i>iso</i> -Acorone	OS	1806	–	–	0.1
Unidentified <sup>h</sup>	–	1844	–	–	11.5
Class composition					
Monoterpene hydrocarbons (MH)	–	–	–	–	2.2
Oxygenated monoterpenes (OM)	–	–	–	–	2.5
Sesquiterpene hydrocarbons (SH)	–	–	–	–	11.4
Oxygenated sesquiterpenes (OS)	–	–	–	–	33.9
Benzenoid compounds (BC)	–	–	–	–	33.9
Aliphatic compound (AC)	–	–	–	–	tr
Total identified, %	–	–	–	–	83.9

<sup>a</sup>Retention indices determined on the DB-5 column using an *n*-alkane homologous series (C<sub>9</sub>–C<sub>24</sub>); <sup>b</sup>retention indices from the literature;<sup>22</sup> <sup>c</sup>retention indices determined on the CP-WAX 52 CB column; <sup>d</sup>peak area calculated on the DB-5 column; <sup>e</sup>*cis/trans* related to methyl vs. isopropyl groups; <sup>f</sup>also known as thymohydroquinone dimethyl ether; tr: trace (<0.05 %); <sup>g</sup>tentative identification based on the comparison of the retention indices with literature values; <sup>h</sup>mass spectrum (70 eV): 234 (M<sup>+</sup>), 219, 173, 145, 117, 93, 91 (100 %), 55, 53