



SUPPLEMENTARY MATERIAL TO  
**Chemical composition and screening of the antimicrobial and  
anti-oxidative activity of extracts of *Stachys* species**

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TABLE I-S. Chemical composition (%) of the extracts of four *Stachys* species

Rf <sup>a</sup>	Compound	Class	Method <sup>b</sup>	S. <i>germanica</i>		S. <i>iva</i>		S. <i>plumosa</i>		S. <i>scardica</i>	
				DE <sup>c</sup>	EA <sup>d</sup>	DE	EA	DE	EA	DE	EA
841	2-Isopropyl-5-methylfuran	O	a,b	– <sup>e</sup>	–	–	–	tr <sup>f</sup>	–	tr	–
939	$\alpha$ -Thujene	T	a,b	–	–	–	–	0.1	–	tr	–
947	$\alpha$ -Pinene	T	a,b,c	–	–	–	0.1	0.1	1.4	0.1	–
969	$\beta$ -Thujene	T	a,b	–	–	–	–	0.1	–	0.1	–
994	$\beta$ -Myrcene	T	a,b	–	–	–	–	–	–	tr	–
996	$\beta$ -Pinene	T	a,b,c	–	–	tr	tr	0.2	0.8	0.1	–
1051	1,8-Cineole	T	a,b,c	0.1	–	–	–	0.1	–	–	–
1098	Terpinolene	T	a,b	–	–	–	–	0.1	–	–	–
1110	$\alpha$ -Pinene epoxide	T	a,b	–	–	–	–	tr	–	–	–
1113	1-Octen-3-yl acetate	FAD	a,b	–	–	–	–	tr	–	–	–
1118	<i>cis</i> -Limonene oxide	T	a,b	–	–	–	–	0.3	–	tr	–
1130	$\alpha$ -Campholenal	T	a,b	–	–	–	–	0.1	–	–	–
1131	Nopinone	T	a,b	–	–	–	–	tr	–	–	–
1140	Camphor	T	a,b,c	0.3	–	–	–	–	–	tr	–
1144	<i>trans</i> -Pinocarveol	T	a,b,c	–	–	–	–	0.3	–	–	–
1149	<i>cis</i> -Verbenol	T	a,b,c	–	–	–	–	0.4	–	0.1	–
1154	Pinocarvone	T	a,b,c	–	–	–	–	0.3	–	–	–
1158	<i>trans</i> -Verbenol	T	a,b,c	–	–	–	–	0.1	–	–	–
1176	Myrtenal	T	a,b,c	–	–	–	–	0.2	–	–	–
1185	Verbenone	T	a,b,c	–	–	–	–	0.4	–	–	–
1192	3-Thujen-10-al	T	a,b	–	–	–	–	0.1	–	–	–

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TABLE I-S. Continued

<i>Rf</i> <sup>a</sup>	Compound	Class	Method <sup>b</sup>	S.		S.		S.		S.	
				<i>germanica</i>		<i>iva</i>		<i>plumosa</i>		<i>scardica</i>	
				DE <sup>c</sup>	EA <sup>d</sup>	DE	EA	DE	EA	DE	EA
1236	Linalyl acetate	T	a,b	–	–	–	–	0.1	–	–	–
1256	Bornyl acetate	T	a,b,c	–	–	–	–	0.1	–	–	–
1319	Bicycloelemene	T	a,b	–	–	0.1	–	–	–	–	–
1321	δ-Elemene	T	a,b	–	–	–	–	–	–	tr	–
1322	Dihydrocarveol acetate <sup>g</sup>	T	a,b	–	–	–	–	tr	–	–	–
1337	α-Cubebene	T	a,b	tr	–	–	–	–	–	0.2	–
1355	Cyclosativene	T	a,b	–	–	0.2	–	–	–	–	–
1361	α-Yangene	T	a,b	–	–	–	–	–	–	0.1	–
1367	α-Copaene	T	a,b	0.5	–	0.9	–	0.1	–	0.3	–
1375	β-Bourbonene	T	a,b	2.2	–	–	–	–	–	0.2	–
1378	β-Cubebene	T	a,b	–	–	–	–	–	–	0.4	–
1380	β-Elemene	T	a,b	–	–	0.2	–	–	–	–	–
1386	1,5-di- <i>epi</i> -β-Bourbonene	T	a,b	tr	–	–	–	–	–	–	–
1392	β-Longipinene	T	a,b	–	–	–	–	–	–	tr	–
1395	Italicene	T	a,b	–	–	–	–	tr	–	–	–
1401	α-Gurjunene	T	a,b	–	–	0.1	–	–	–	–	–
1402	6- <i>epi</i> -α-Cubebene	T	a,b	–	–	–	–	–	–	tr	–
1409	β-Caryophyllene	T	a,b,c	0.7	–	0.9	tr	0.1	–	1.3	tr
1418	β-Copaene	T	a,b	0.2	–	–	–	–	–	0.2	–
1422	Calarene	T	a,b	–	–	–	–	–	–	0.1	–
1429	Aromadendrene	T	a,b	–	–	–	–	–	–	0.2	–
1432	Isogermacrene D	T	a,b	0.2	–	0.1	–	–	–	–	–
1440	α-Humulene	T	a,b,c	–	–	0.2	–	0.1	–	0.1	–
1448	<i>cis</i> -Muurolo-4(15),5-diene	T	a,b	0.3	–	0.1	–	0.1	–	0.1	–
1452	<i>trans</i> -β-Ionone-5,6-epoxide	CR	a,b	–	–	0.1	–	0.1	–	tr	–
1454	( <i>E</i> )-β-Farnesene	T	a,b	0.3	–	tr	–	–	–	–	–
1457	( <i>E</i> )-β-Ionone	CR	a,b	–	–	–	–	0.2	–	–	–
1459	<i>epi</i> -( <i>E</i> )-β-Caryophyllene	T	a,b	–	–	0.2	–	–	–	–	–
1459	γ-Muurolole	T	a,b	0.6	–	–	–	–	–	2.0	–
1463	<i>ar</i> -Curcumene	T	a,b	–	–	–	–	0.2	–	–	–
1464	Germacrene D	T	a,b,c	1.5	–	0.3	–	–	–	–	–
1469	<i>cis</i> -β-Guaiene	T	a,b	–	–	–	–	–	–	0.2	–
1475	γ-Amorphene	T	a,b	–	–	–	–	–	–	0.6	–
1476	<i>epi</i> -Cubebol	T	a,b	–	–	0.4	–	–	–	tr	–
1482	β-Curcumene	T	a,b	tr	–	–	–	–	–	–	–
1491	γ-Cadinene	T	a,b	–	–	–	–	–	–	2.0	–
1492	Cubebol	T	a,b	–	–	0.9	–	–	–	–	–
1495	<i>cis</i> -Calamenene	T	a,b	–	–	–	–	–	–	tr	–
1498	δ-Cadinene	T	a,b	–	–	2.7	–	0.2	–	1.4	–
1510	Dihydroactinidiolide	CR	a,b	–	–	–	–	0.3	–	–	–
1518	α-Calacorene	T	a,b	–	–	–	–	–	–	0.7	–
1539	α-Agarofuran	T	a,b	–	–	–	–	–	–	0.5	0.1
1542	β-Calacorene	T	a,b	–	–	–	–	–	–	0.6	–
1554	1,8-Oxidocadin-4-ene	T	a,b	–	–	–	–	0.1	–	–	–

TABLE I-S. Continued

<i>R</i> <sup>a</sup>	Compound	Class	Method <sup>b</sup>	S.		S.		S.		S.	
				<i>germanica</i>		<i>iva</i>		<i>plumosa</i>		<i>scardica</i>	
				DE <sup>c</sup>	EA <sup>d</sup>	DE	EA	DE	EA	DE	EA
1563	Spathulenol	T	a,b,c	3.8	–	3.8	–	–	–	0.4	–
1571	Caryophyllene oxide	T	a,b,c	4.3	–	3.6	0.1	0.7	–	3.1	–
1580	4(14)-Salvialen-1-one	T	a,b	1.4	–	–	–	–	–	1.3	–
1583	Viridiflorol	T	a,b	2.5	–	1.1	–	–	–	–	–
1587	$\beta$ -Oplopenone	T	a,b	–	–	–	–	0.4	–	–	–
1597	Humulene epoxide II	T	a,b	–	–	–	–	–	–	0.5	–
1601	Copaborneol	T	a,b	–	–	2.0	–	–	–	–	–
1603	<i>epi</i> -Marsupellol	T	a,b	–	–	–	–	–	–	0.1	–
1608	1,10-di- <i>epi</i> -Cubenol	T	a,b	–	–	–	–	–	–	0.5	–
1623	Isospathulenol	T	a,b	–	–	–	–	–	–	1.9	–
1625	1- <i>epi</i> -Cubenol	T	a,b	–	–	1.2	–	–	–	–	–
1632	10- <i>epi</i> -Italicen-4-one	T	a,b	–	–	–	–	–	–	0.3	–
1637	$\tau$ -Muurolol	T	a,b	0.3	–	1.2	–	0.3	–	1.6	–
1651	$\alpha$ -Cadinol	T	a,b	0.5	–	–	–	0.2	–	2.1	–
1660	10 $\beta$ -Hydroxy- <i>cis</i> -calamenene	T	a,b	–	–	–	–	0.1	–	–	–
1665	10 $\alpha$ -Hydroxy- <i>cis</i> -calamenene	T	a,b	–	–	–	–	0.1	–	0.4	–
1669	Valeranone	T	a,b	2.1	–	1.4	0.1	–	–	–	–
1675	3-Oxo- $\alpha$ -damascone	CR	a,b	–	–	–	–	0.2	–	–	–
1678	Cadalene	T	a,b	–	–	–	–	–	–	1.9	–
1687	Germacre-4(15),5,10(14)-trien-1-al	T	a,b	–	–	0.2	–	–	–	–	–
1690	2,3-Dihydrofarnesol	T	a,b	–	–	0.7	–	–	–	–	–
1692	3-Hydroxy-5,6-epoxy- $\beta$ -ionone	CR	a,b	1.5	–	–	–	0.5	–	–	–
1714	(2 <i>E</i> ,6 <i>E</i> )-Farnesol	T	a,b	–	–	0.3	–	–	–	–	–
1731	7,8-Dihydro-3-oxo- $\alpha$ -ionol	CR	a,b	1.0	–	–	–	–	–	0.3	–
1766	Methyl (2 <i>E</i> ,6 <i>E</i> )-farnesate	T	a,b	0.5	–	–	–	–	–	–	–
1779	( <i>Z</i> )-7-Hexadecenal	FAD	a,b	–	–	tr	–	0.1	–	–	–
1785	( <i>E</i> )-7-Hexadecenal	FAD	a,b	–	–	–	–	0.1	–	–	–
1794	Antracene	O	a,b	–	–	–	–	0.2	–	0.3	–
1803	(2 <i>Z</i> ,6 <i>E</i> )-Farnesyl acetate	T	a,b	–	–	0.1	–	0.1	–	–	–
1823	Hexadecanal	FAD	a,b	–	–	–	–	0.3	–	–	–
1844	Neophytadiene, isomer I	T	a,b	–	1.1	1.4	0.3	2.7	0.6	2.6	2.8
1845	Hexahydrofarnesylacetone	CR	a,b	3.5	–	–	–	–	–	–	–
1865	Neophytadiene, isomer II	T	a,b	–	0.2	0.1	–	0.3	–	0.3	0.2
1869	( <i>E</i> )-Nuciferyl acetate	T	a,b	0.8	–	0.2	–	–	–	–	–
1880	Neophytadiene, isomer III	T	a,b	0.5	0.4	0.5	0.1	0.6	–	0.5	0.6
1890	( <i>Z</i> )-Nuciferyl propionate	T	a,b	–	–	0.1	–	–	–	–	–
1900	Nonadecane	FAD	a,b,c	1.2	–	0.3	–	0.1	–	0.2	–
1902	Farnesyl acetone	CR	a,b	–	0.4	–	–	–	–	–	–
1905	Isopimara-8,15-diene	T	a,b	–	–	–	–	0.2	–	–	–

TABLE I-S. Continued

<i>R</i> <sup>a</sup>	Compound	Class	Method <sup>b</sup>	S.		S.		S.		S.	
				<i>germanica</i>		<i>iva</i>		<i>plumosa</i>		<i>scardica</i>	
				DE <sup>c</sup>	EA <sup>d</sup>	DE	EA	DE	EA	DE	EA
1910	Methyl hexadecanoate ( <i>syn.</i> <sup>h</sup> methyl palmitate)	FAD	a,b	1.2	0.2	0.1	–	0.3	–	0.5	–
1922	Cembrene	T	a,b	–	–	0.2	–	–	–	–	–
1929	1-Methylphenanthrene	O	a,b	–	–	–	–	–	1.2	–	–
1940	Isophytol	T	a,b	–	–	–	–	tr	–	0.3	–
1944	( <i>Z</i> )-Nuciferyl isobutyrate	T	a,b	4.5	0.2	15.3	1.2	0.1	–	–	–
1965	Labda-7,13(16),14-triene	T	a,b	–	–	0.2	–	–	–	–	–
1968	<i>n</i> -Hexadecanoic acid	FAD	a,b,c	–	–	–	–	6.0	–	–	–
1979	Ethyl hexadecanoate ( <i>syn.</i> Ethyl palmitate)	FAD	a,b	1.7	0.1	0.3	–	6.1	–	4.8	–
2000	Eicosane	FAD	a,b,c	0.5	–	–	–	–	–	1.9	–
2001	Octadecanal ( <i>syn.</i> stearaldehyde)	FAD	a,b	–	–	–	0.1	–	–	–	0.1
2007	13- <i>epi</i> -Manoyl oxide	T	a,b	–	–	–	–	2.4	–	–	–
2013	Methyl heptadecanoate	FAD	a,b	–	–	0.1	–	–	–	0.9	–
2039	Abieta-8,11,13-triene	T	a,b	0.3	–	0.1	–	13.6	17.8	5.0	0.8
2054	( <i>Z</i> )-Nuciferyl isovalerate	T	a,b	0.9	–	0.4	–	–	–	–	–
2073	Methyl-( <i>Z,Z,Z</i> )-9,12,15- -octadecatrienoate ( <i>syn.</i> methyl linolenate)	FAD	a,b	1.5	–	0.1	–	1.1	–	0.8	–
2076	( <i>Z</i> )-Nuciferyl 2-methylbutyrate	T	a,b	0.9	–	0.1	–	–	–	–	–
2079	Methyl-( <i>Z,Z</i> )-9,12-octa- decenoate ( <i>syn.</i> methyl linoleate)	FAD	a,b	–	0.4	–	–	–	–	–	–
2083	( <i>Z</i> )-9-Octadecenoic acid ( <i>syn.</i> Oleic acid)	FAD	a,b	–	0.6	–	–	1.7	–	0.2	0.5
2084	Methyl-( <i>Z</i> )-9-octade- cenoate ( <i>syn.</i> methyl oleate)	FAD	a,b	1.0	–	0.2	–	–	–	0.4	–
2093	Isoabienol	T	a,b	–	–	3.6	1.2	–	–	–	–
2100	Heneicosane	FAD	a,b,c	2.2	0.4	–	0.4	0.2	–	0.5	0.1
2105	<i>trans</i> -Phytol	T	a,b	5.2	0.7	4.0	0.8	7.9	–	3.8	0.9
2127	Methyl octadecanoate ( <i>syn.</i> Methyl stearate)	FAD	a,b	1.5	–	3.2	–	0.4	0.9	0.4	0.1
2140	Ethyl ( <i>Z,Z</i> )-9,12-octa- decadienoate ( <i>syn.</i> ethyl linoleate)	FAD	a,b	1.4	–	0.3	–	2.9	–	0.4	–
2145	Ethyl ( <i>Z,Z,Z</i> )-9,12,15-oc- tadecatrienoate ( <i>syn.</i> ethyl linolenate)	FAD	a,b	0.5	–	0.3	–	4.4	–	0.2	–
2151	Ethyl ( <i>Z</i> )-9-octadecenoate ( <i>syn.</i> ethyl oleate)	FAD	a,b	0.8	0.4	0.6	0.4	–	–	0.2	–
2170	Thunbergol	T	a,b	–	–	–	–	2.3	–	0.9	–
2170	Abieta-8(14),13(15)-diene	T	a,b	–	–	0.2	–	–	–	–	–

TABLE I-S. Continued

<i>R</i> <sup>a</sup>	Compound	Class	Method <sup>b</sup>	S.		S.		S.		S.	
				<i>germanica</i>		<i>iva</i>		<i>plumosa</i>		<i>scardica</i>	
				DE <sup>c</sup>	EA <sup>d</sup>	DE	EA	DE	EA	DE	EA
2178	Ethyl octadecanoate	FAD	a,b	0.2	–	0.2	–	1.5	–	0.4	–
2200	Docosane	FAD	a,b,c	1.6	0.6	0.3	tr	–	–	0.6	0.2
2209	Sclareol	T	a,b	–	–	0.3	0.1	–	1.5	–	–
2223	<i>cis</i> -Totarol	T	a,b	–	–	–	0.9	3.0	–	–	–
2266	2-Methyldocosane	FAD	a,b	–	0.7	–	–	–	–	–	–
2270	Dehydroabietal	T	a,b	–	–	–	–	3.5	–	0.9	–
2271	1-Eicosanol	FAD	a,b	2.8	0.4	–	–	–	–	–	–
2274	3-Methyldocosane	FAD	a,b	–	–	–	0.4	–	–	–	–
2300	Tricosane	FAD	a,b,c	5.5	1.8	3.8	0.5	6.6	–	17.6	1.4
2328	11-Methyltricosane	FAD	a,b	–	–	–	–	–	–	–	4.4
2329	$\delta$ -Eicosanolactone	FAD	a,b	–	–	0.5	0.3	0.7	–	0.7	–
	( <i>syn.</i> meadowlactone)										
2338	Dehydroabietic acid methyl ester	T	a,b	–	–	–	–	2.8	–	1.4	1.2
2347	Dehydroabietol	T	a,b	–	–	–	–	1.3	6.2	–	–
2361	Butyl octadecanoate	FAD	a,b	–	–	0.5	0.2	1.4	–	0.8	–
2365	2-Methyltricosane	FAD	a,b	–	0.2	–	–	–	–	–	–
2378	Ethyl eicosanoate	FAD	a,b	0.6	–	tr	–	0.4	–	2.1	–
2398	Labd-13( <i>E</i> )-en-8 $\alpha$ ,15-diol	T	a,b	–	–	14.3	–	–	–	–	–
2400	Tetracosane	FAD	a,b,c	1.0	0.6	tr	–	0.9	–	0.8	0.5
2408	Methyl heneicosanoate	FAD	a,b	–	–	–	–	0.6	–	0.5	–
2431	Methyl neoabietate	T	a,b	–	–	0.3	9.6	0.2	–	–	–
2465	2-Methyltetracosane	FAD	a,b	–	–	–	0.7	–	–	0.4	0.3
2468	1-Docosanol	FAD	a,b	1.2	0.4	–	–	–	–	–	–
2474	3-Methyltetracosane	FAD	a,b	–	0.3	–	–	–	–	–	–
2500	Pentacosane	FAD	a,b,c	3.6	2.5	0.6	0.8	1.2	2.6	1.3	1.4
2544	Tricosanoic acid	FAD	a,b	–	–	–	–	–	–	0.3	–
2564	2-Methylpentacosane	FAD	a,b	0.1	–	–	–	–	13.2	–	–
2573	3-Methylpentacosane	FAD	a,b	–	0.3	–	1.5	–	–	–	–
2576	Ethyl docosanoate	FAD	a,b	–	–	–	–	0.8	6.1	0.2	–
2600	Hexacosane	FAD	a,b,c	0.3	–	0.2	–	0.3	–	0.2	0.7
2615	3,7-Dimethylpentacosane	FAD	a,b	–	0.1	–	–	–	–	–	–
2636	10-Methylhexacosane	FAD	a,b	–	–	–	–	–	–	–	0.6
2664	2-Methylhexacosane	FAD	a,b	–	–	–	–	0.1	–	0.4	–
2667	2,6,10,15,19,23-Hexamethyltetracosane (squalane)	T	a,b	0.2	–	–	–	–	–	0.6	0.2
2674	3-Methylhexacosane	FAD	a,b	–	0.5	–	–	–	–	–	–
2700	Heptacosane	FAD	a,b,c	4.9	7.2	2.9	5.3	4.3	27.7	4.3	5.0
2771	3-Methylheptacosane	FAD	a,b	0.2	1.0	–	0.1	0.1	–	–	–
2800	Octacosane	FAD	a,b,c	0.8	1.9	0.8	1.4	0.5	2.8	0.3	1.1
2808	Squalene	T	a,b	0.8	1.1	0.1	0.2	0.2	–	0.5	1.6
2835	10-Methyloctacosane	FAD	a,b	–	0.2	–	–	–	–	–	–
2864	2-Methyloctacosane	FAD	a,b	–	0.4	–	0.7	–	–	–	–

TABLE I-S. Continued

Compound	Class	Method <sup>b</sup>	S.		S.		S.		S.		
			<i>germanica</i>		<i>iva</i>		<i>plumosa</i>		<i>scardica</i>		
			DE <sup>c</sup>	EA <sup>d</sup>	DE	EA	DE	EA	DE	EA	
2859	10-Demethylsqualene	T	a,b	0.1	0.2	0.5	–	0.3	–	1.0	0.4
2900	Nonacosane	FAD	a,b,c	17.0	36.9	18.0	28.3	–	6.5	3.6	19.3
2934	10-Methylnonacosane	FAD	a,b	–	2.7	–	12.0	–	–	–	–
2973	3-Methylnonacosane	FAD	a,b	–	0.3	–	–	–	3.2	–	0.6
3000	Triacotane	FAD	a,b,c	0.6	2.1	–	2.1	–	3.6	8.0	5.9
3033	10-Methyltriacotane	FAD	a,b	–	0.3	–	–	–	0.5	–	–
3038	3,7,15-Trimethyl- nonacosane	FAD	a,b	–	0.1	–	–	–	0.1	–	–
3100	Hentriacotane	FAD	a,b	–	20.9	–	23.3	–	–	–	43.7
Total				96.4	88.8	98.1	93.2	91.9	96.7	97.5	94.7
Yield, mass %				1.4	10.0	1.5	4.0	1.4	8.0	1.5	5.8
Grouped components											
Terpenoids (T)				36.5	3.9	64.7	14.7	47.3	28.3	43.0	8.8
Monoterpene hydrocarbons				–	–	tr	0.1	0.6	2.2	0.3	–
Oxygenated monoterpenes				0.4	–	–	–	2.5	–	0.1	–
Sesquiterpene hydrocarbons				6.5	–	6.0	tr	0.8	–	12.6	tr
Oxygenated sesquiterpenes				22.5	0.2	32.9	1.4	2.1	–	12.7	0.1
Diterpenes				6.0	2.4	25.2	13.0	40.8	26.1	15.7	6.5
Triterpenes				1.1	1.3	0.6	0.2	0.5	–	2.1	2.2
Fatty acid derived compounds (FAD)				59.9	84.9	33.4	78.5	44.6	68.4	54.5	85.9
<i>n</i> -Alkanes				39.2	74.9	26.9	62.1	14.1	43.2	39.3	79.3
Branched alkanes				0.3	7.1	–	15.4	0.2	17.0	0.8	5.9
Alcohols				4.0	0.8	–	–	–	–	–	–
Aldehydes				–	–	tr	0.1	0.5	–	–	0.1
Fatty acids and fatty acid esters				10.4	1.7	6.4	0.9	28.3	7.0	13.8	0.6
Carotenoid derived compounds				6.0	0.4	0.1	–	1.3	–	0.3	–
Others (O)				–	–	–	–	0.2	1.2	0.3	–

<sup>a</sup>Components listed in order of elution from an SPB-1 column (*RI* – experimentally determined retention indices on the mentioned column by co-injection of a homologous series of *n*-alkanes C<sub>8</sub>–C<sub>31</sub>); <sup>b</sup>a – constituent identified by retention index matching; <sup>b</sup>b – constituent identified by mass spectra comparison; <sup>c</sup>c – constituent identified by co-injection of an authentic sample; <sup>c</sup>d – diethyl ether extract; <sup>d</sup>d – ethyl acetate extract; <sup>e</sup>e – not detected; <sup>f</sup>f – trace (<0.05 %); <sup>g</sup>g – correct stereoisomer not determined; <sup>h</sup>h – synonym