

Supporting Information to

Biodiversity within *Melissa officinalis*: Variability of Bioactive Compounds in a Cultivated Collection

Table S1: Oil yield in leaves and stems of lemon balm, *Melissa officinalis* ssp. *officinalis* (MOFF) and *M. officinalis* ssp. *altissima* (MALT), ($\mu\text{g/g}$, calculated from the FID signal)

Table S2: Composition of the leaf essential oils from *Melissa officinalis* (% of total peak area on a apolar HP5-MS column, calculated from the FID signal)

Table S3: Composition of the stem essential oils from *Melissa officinalis* (% of total peak area on a apolar HP5-MS column, calculated from the FID signal)

Figure S1: *Melissa officinalis*: composition of the leaf essential oils from the 1st cut

Figure S2: *Melissa officinalis*: composition of the leaf essential oils from the 2nd cut

Figure S3: *Melissa officinalis*: composition of the stem essential oils from the 1st cut

Figure S4: *Melissa officinalis*: composition of the stem essential oils from the 2nd cut

Table S1: Oil yield in leaves and stems of lemon balm, *Melissa officinalis* ssp. *officinalis* (MOFF) and *M. officinalis* ssp. *altissima* (MALT), ($\mu\text{g/g}$, calculated from the FID signal)

Accession	1 st cut	2 nd cut	1 st cut	2 nd cut
Leaves		Stems		
MOFF				
M1	5083	7180	14.1	50.4
M2	1150	5652		
M4	3210	12245	8.2	1612
M5	845	4753		
M6	1937	6512		
M7	414	6745		
M8	893	8995		
M10	1539	6311	14.2	82.3
M11	667	6902		
M13	293	5234		
M16	843	6158		
M25	554	8968		
M26	782	12669	24.6	634
M27	335	8358	36.5	54.6
M29	627	8062		
MALT				
M9	807	-		
M12	167	2731	8.0	38.4
M14	59	1634		
M15	76	1033		
M17	389	3212	14.0	93.1
M18	139	1313		
M19	100	996		
M20	117	1081	15.3	85.7
M21	164	2220	0.1	45.4
M22	128	2759	0.4	81.3
M23	84	1531		
M24	68	909		
M28	129	947		

Table S2: Composition of the leaf essential oils from *Melissa officinalis* (% of total peak area on a apolar HP5-MS column, calculated from the FID signal)

Compound	RI	subsp. <i>officinalis</i> MOFF				subsp. <i>altissima</i> MALT			
		1 st cut		2 nd cut		1 st cut		2 nd cut	
		mean*	SD	mean*	SD	mean*	SD	mean*	SD
<i>trans</i> -2-Hexenal	856	<0.05	<0.1	0.1	0.1	0.2	0.5	<0.05	
α -Thujene	933			<0.05		0.1	0.2	0.8	0.4
α -Pinene	942			<0.05		0.5	1.3	5.0	2.9
Camphene	956							0.1	0.1
1-Octen-3-ol	981	0.3	0.2	0.2	0.1	0.3	0.8		
Sabinene	982			0.1	0.4	1.6	3.6	14.7	8.3
β -Pinene	986			0.1	0.4	1.5	3.1	11.9	5.8
6-Methyl-5-heptene-2-one	989	0.3	0.1	0.5	0.2	0.5	1.1		
Myrcene	994	<0.05		0.2	<0.1	<0.05		0.4	0.2
α -Terpinen	1022					0.1	0.2	0.5	0.3
<i>p</i> -Cymene	1031					<0.05		0.1	0.1
Limonene	1036					0.1	0.3	1.3	0.6
β -Phellandrene	1036								
1,8-Cineol	1038							0.3	0.1
<i>Z</i> - β -Ocimene	1042	<0.05		<0.05		0.1	0.3	0.4	0.1
<i>E</i> - β -Ocimene	1053	0.6	0.4	0.2	0.1	0.3	0.5	1.4	0.5
2,6-Dimethyl hept-5-en-1-al	1059	0.2	0.1						
γ -Terpinene	1065					0.2	0.5	1.3	0.5
Terpinolene	1093			<0.05		<0.05		0.3	0.1
Linalool	1102	0.7	0.3	0.3	0.2	0.1	0.2	0.1	0.2
<i>cis</i> -Roseoxide	1115	0.1	0.1						
<i>trans</i> -Roseoxide	1133	0.1	0.1						
α -Campholenaldehyd	1133	<0.05				<0.05		0.1	<0.1
Photocitral	1147	0.1	0.1	0.1	<0.1				
<i>trans</i> -Pinocarveol	1148					0.2	0.4	0.3	0.1
<i>exo</i> -Isocitral	1150	0.2	0.1	0.3	<0.1				
Isopulegol	1154	0.1	0.1			<0.05			
Citronellal	1160	20.6	8.4	0.8	0.3	0.5	1.0	0.3	0.2
<i>iso</i> -Isopulegol	1166	0.1	0.1						
<i>Z</i> -Isocitral	1170	1.3	0.3	1.4	0.2				
Pinocarpone	1172					0.1	0.2	0.2	0.1
Rosefuran epoxide	1180	<0.05		0.1	0.1				
Terpinen-4-ol	1185							1.2	0.5
<i>E</i> -Isocitral	1187	1.8	0.4	2.0	0.2	0.2	0.6		
α -Terpineol	1196					0.1	0.5	0.1	0.1
Myrtenal	1204					0.2	0.6	0.4	0.1
Citronellol	1235	0.2	0.2	<0.05					
Neral	1253	19.9	5.1	35.0	1.6	0.4	1.0	0.4	0.5
Geranyl formate	1262	0.1	0.1	0.1	0.1				

Table S2: continued

Compound	RI	subsp. <i>officinalis</i>				subsp. <i>altissima</i>			
		1 st cut		2 nd cut		1 st cut		2 nd cut	
		mean*	SD	mean*	SD	Mean*	SD	Mean*	SD
Methyl citronellate	1265	1.1	0.5	<0.05					
Geranial	1283	30.8	7.0	51.3	2.6	0.7	1.8	0.6	0.8
Methyl geranate	1328	0.3	0.1	0.2	0.2				
Geranic acid	1357	<0.05		0.1	0.4	0.2	0.7		
α -Copaene	1386	0.5	0.4	1.0	0.4	3.5	2.4	1.7	1.2
β -Bourbonene	1397	<0.05				0.7	0.4	0.2	0.1
β -Elemene	1400	0.2	0.3			1.3	0.7	1.0	0.4
β -Caryophyllene	1432	4.0	2.8	3.1	1.1	9.9	3.0	17.2	6.9
β -Gurjunene	1442							0.1	<0.1
<i>E</i> - β -Farnesene	1462	0.1	0.1	<0.05		<0.05			
α -Humulene	1469	0.3	0.2	0.2	0.1	0.6	0.4	1.1	0.4
9- <i>epi-E</i> -Caryophyllene	1477	<0.05		<0.05		0.6	0.6	2.5	1.6
α -Amorphene	1489							0.2	0.1
Germacrene D	1492	1.2	1.9	0.2	0.2	15.4	12.5	19.6	7.1
<i>Z,E</i> - α -Farnesene	1498	0.2	0.5	<0.05					
γ -Amorphene	1505							0.2	0.1
Bicyclogermacrene	1507							0.2	0.4
<i>E,E</i> - α -Farnesene	1513	0.1	0.2	<0.05		0.5	0.5	0.5	0.4
γ -Cadinene	1529	<0.05				0.3	0.3	0.2	0.1
δ -Cadinene	1536	0.3	0.3	<0.05		1.2	0.6	0.8	0.7
MW 220**	1569	0.5	0.2	<0.05		2.8	1.2	0.7	0.4
Spathulenol	1592							0.1	0.1
Caryophyllenoxide	1600	9.2	3.6	1.3	0.6	36.6	12.9	7.1	3.0
MW 220**	1627	0.6	0.2	0.1	0.1	1.4	0.9	0.4	0.1
Caryophylla-4(12),8(13)-dien-5ol	1654	0.1				0.5	0.5	0.2	0.2
α -Cadinol	1670	0.3	0.3	<0.05	0.1	0.8	1.0	0.9	0.7
MW 220**	1686	0.5	0.2			3.2	0.8	0.5	0.2
MW 220**	1702	0.1	0.1			0.4	0.6	0.3	0.1
2 <i>E,6E</i> -Farnesal	1750							0.1	0.1
Hexahydrofarnesylacetone	1849	0.1	0.1			0.1	0.2	0.1	0.1
Hexadecanoic acid	1960	0.6	0.3	<0.05		2.6	2.1	0.1	0.1

* Mean of the accessions and standard deviation (SD), n=15 for MOFF and n=13 for MALT, ** oxidised sesquiterpene with molar mass 220

Table S3: Composition of the stem essential oils from *Melissa officinalis* (% of total peak area on a apolar HP5-MS column, calculated from the FID signal)

Compound	RI	subsp. <i>officinalis</i> MOFF				subsp. <i>altissima</i> MALT			
		1 st cut		2 nd cut		1 st cut		2 nd cut	
		mean*	SD	mean*	SD	mean*	SD	mean*	SD
α -Thujene	933							0.5	0.1
α -Pinene	942			<0.1	0.1	0.5	1.1	2.0	1.8
Sabinene	982			0.1	0.2	0.7	1.5	5.3	3.9
β -Pinene	986			0.1	0.2	1.0	2.3	5.7	3.9
6-Methyl-5-heptene-2-one	989			0.1	0.2				
Myrcene	994	0.1	0.2	0.1	0.1			0.1	0.2
α -Terpinen	1022							0.5	0.5
<i>p</i> -Cymene	1031							<0.1	0.1
Limonene	1036							0.4	0.4
β -Phellandrene	1036								
1,8-Cineol	1038							<0.05	0.1
<i>Z</i> - β -Ocimene	1042							<0.05	0.1
<i>E</i> - β -Ocimene	1053	0.1	0.2	<0.05	<0.05			0.3	0.2
γ -Terpinene	1065					0.4	1.0	1.4	0.9
Terpinolene	1093							0.3	0.3
Linalool	1102			0.1	0.1				
<i>trans</i> -Roseoxide	1133	0.7	0.8						
<i>exo</i> -Isocitral	1150			0.2	0.1				
Citronellal	1160	9.8	7.1	1.1	0.9				
<i>Z</i> -Isocitral	1170			1.1	0.3				
Pinocarvone	1172							0.1	0.1
Rosefuran epoxide	1180	1.6	3.6	1.3	2.7	1.5	2.3		
Terpinen-4-ol	1185							0.4	0.4
Myrtenal	1204							0.1	0.1
Neral	1253	8.0	2.7	23.6	6.5			0.1	0.3
Geranial	1283	14.5	5.5	44.7	11.0			0.2	0.5
Methyl geranate	1328	0.1	0.2	0.5	0.3				
α -Copaene	1386	11.3	4.2	6.7	1.7	2.1	3.5	1.7	2.6
β -Bourbonene	1397			<0.05	0.1	0.5	0.7	0.7	0.4
β -Elemene	1400	0.1	0.3	0.1	0.2	0.6	0.9	1.4	0.2
β -Caryophyllene	1432	16.3	4.0	6.9	5.0	7.8	7.7	19.0	9.0
β -Gurjunene	1442							0.2	0.1
α -Humulene	1469	0.6	0.5	0.4	0.3	0.2	0.5	1.2	0.6
9- <i>epi-E</i> -Caryophyllene	1477			0.2	0.4			0.8	1.0
α -Amorphene	1489							0.2	0.2
Germacrene D	1492	1.9	0.9	1.9	3.3	49.6	34.4	31.6	8.2
Bicyclogermacrene	1507							0.9	0.6
δ -Cadinene	1536	0.2	0.4	0.1	0.2	0.4	0.5	0.7	0.1
MW 220**	1569	0.7	0.9						
Spathulenol	1592					1.3	1.2		

Table S3: continued

Compound	RI	subsp. <i>officinalis</i> MOFF				subsp. <i>altissima</i> MALT			
		1 st cut		2 nd cut		1 st cut		2 nd cut	
		mean*	SD	mean*	SD	mean*	SD	mean*	SD
Caryophyllenoxide	1600	24.3	6.4	4.6	2.8	26.6	18.3	14.8	4.3
Caryophylla-4(12),8(13)-dien-5ol	1654			0.4	0.3			0.9	0.8
α -Cadinol	1670			0.3	0.4	0.2	0.5	0.8	0.3
MW 220**	1702			0.1	0.3	0.3	0.7	0.9	0.9
Hexahydrofarnesylacetone	1849	1.1	0.7	0.3	0.2				
Hexadecanoic acid	1960	0.4	1.0						

* Mean of the accessions and standard deviation (SD), n = 5, ** oxidised sesquiterpene with molar mass 220

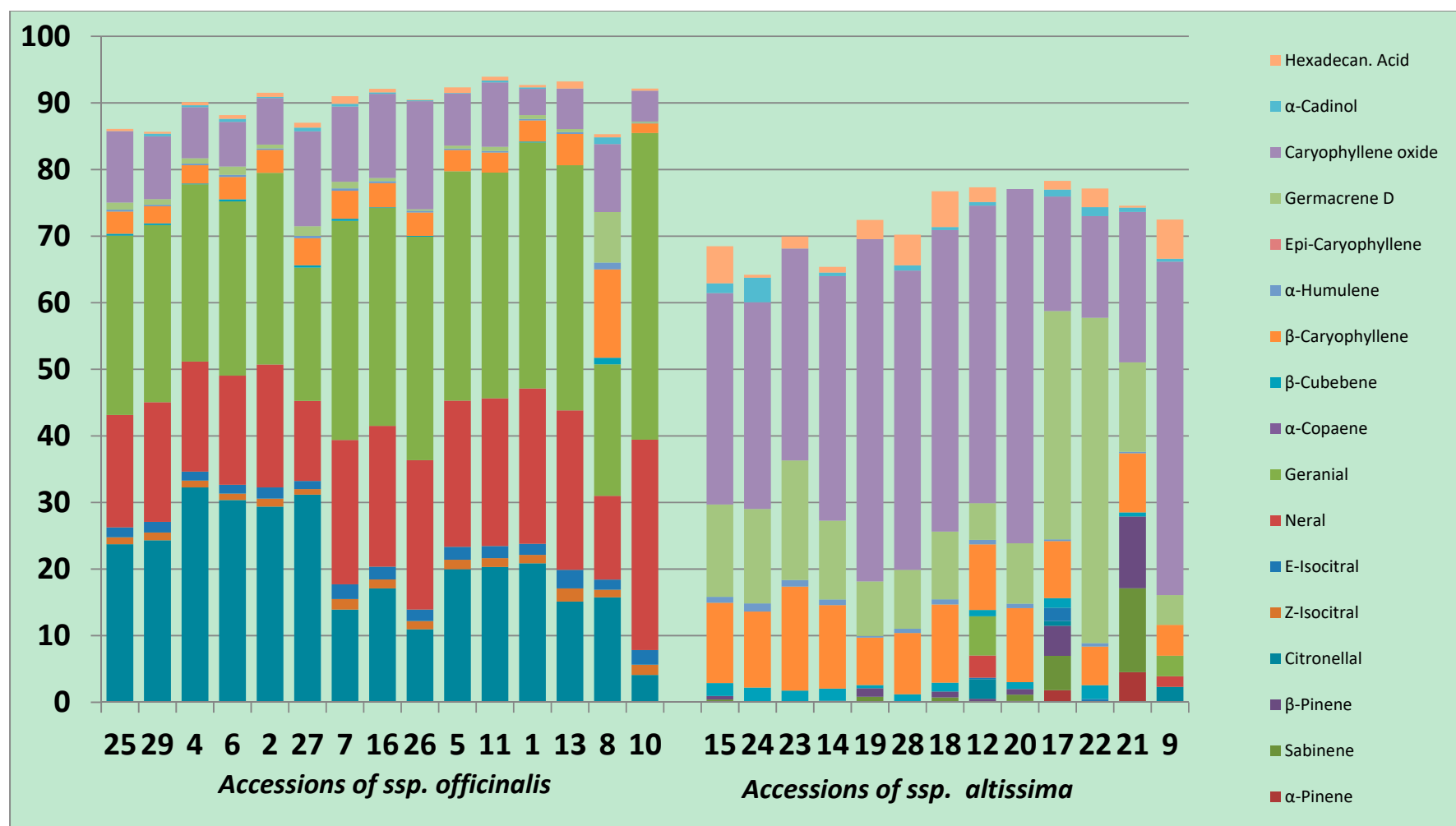


Figure S1: *Melissa officinalis*: composition of the leaf essential oils from the 1st cut

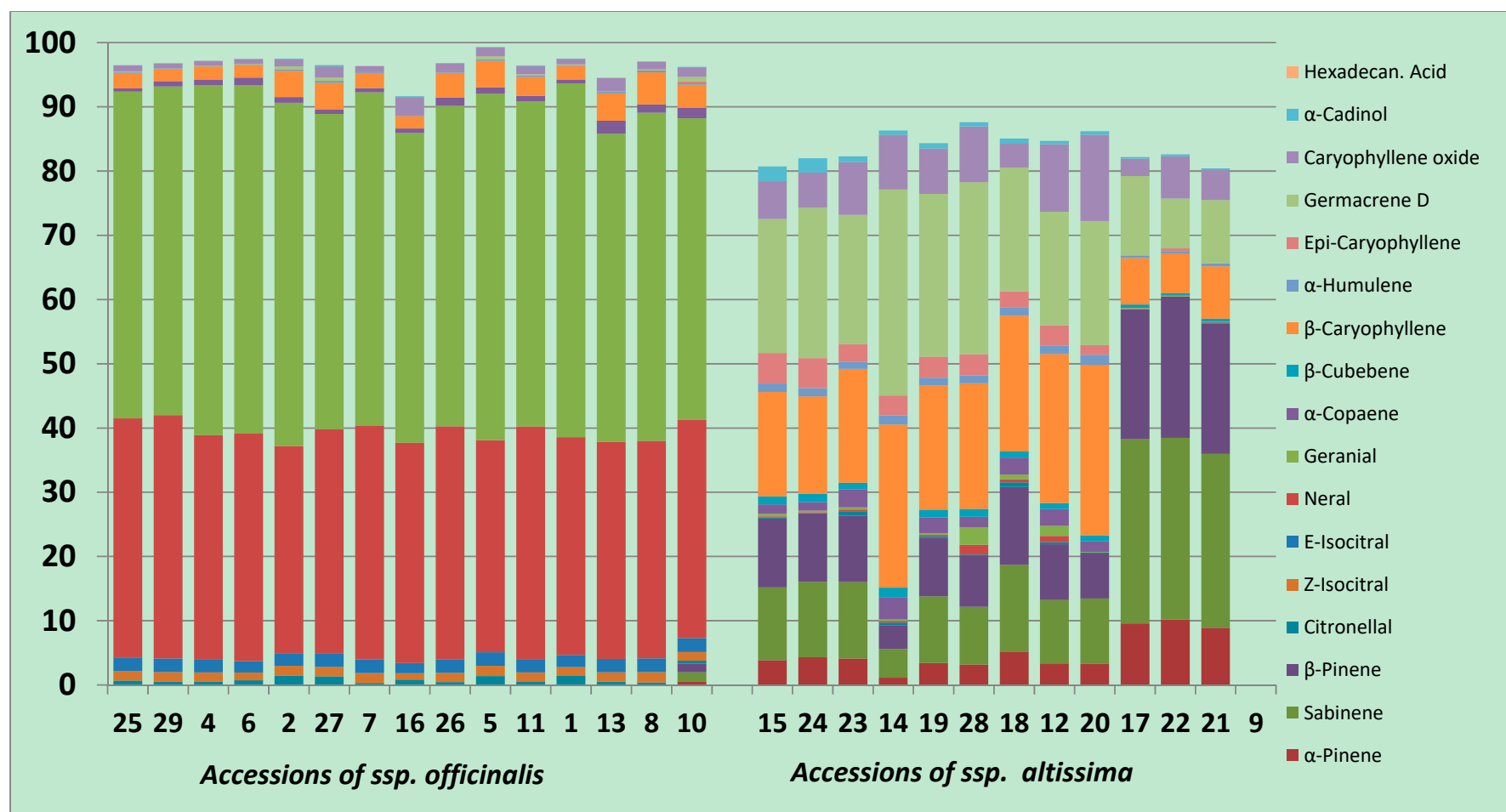


Figure S2: *Melissa officinalis*: composition of the leaf essential oils from the 2nd cut

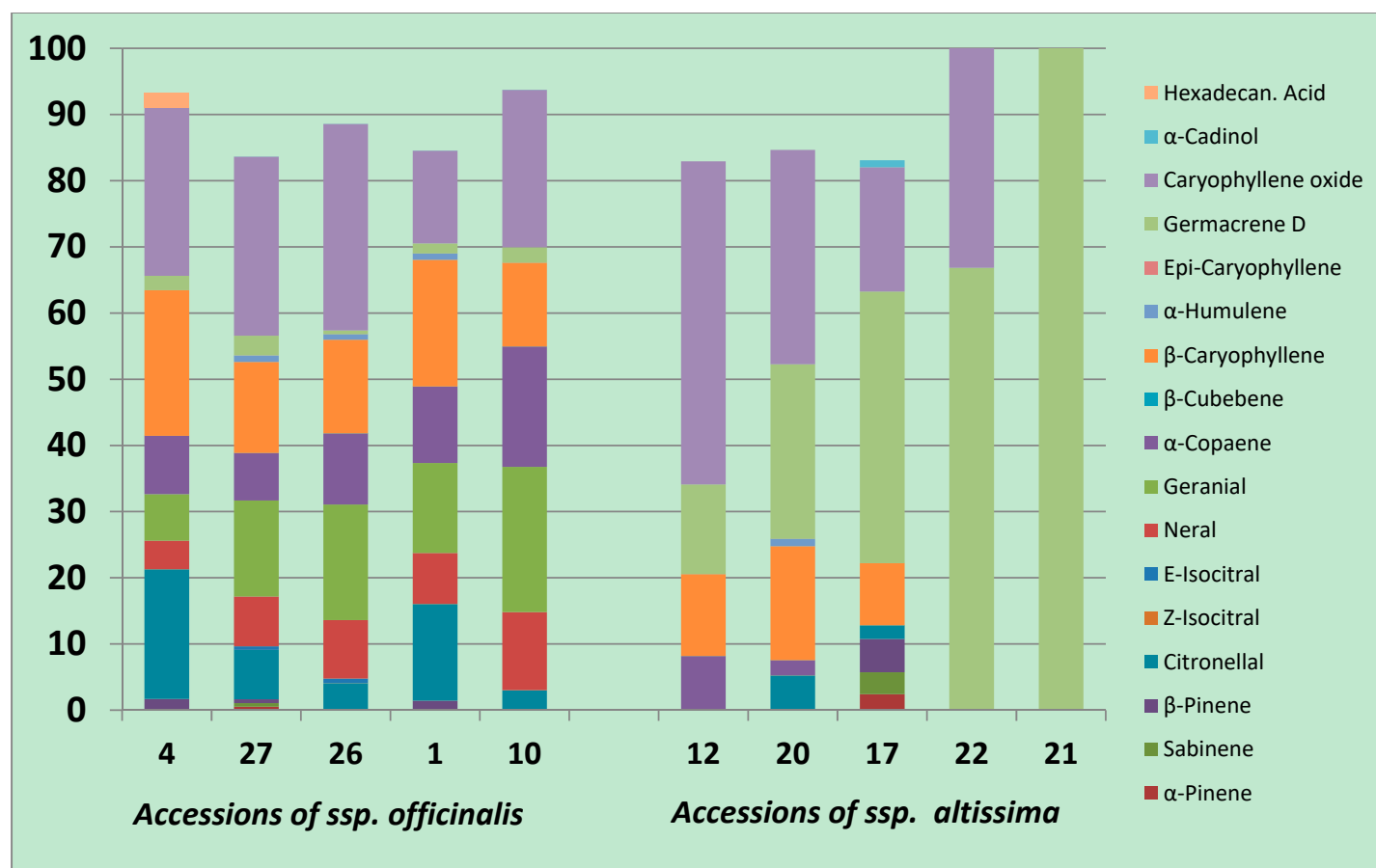


Figure S3: *Melissa officinalis*: composition of the stem essential oils from the 1st cut

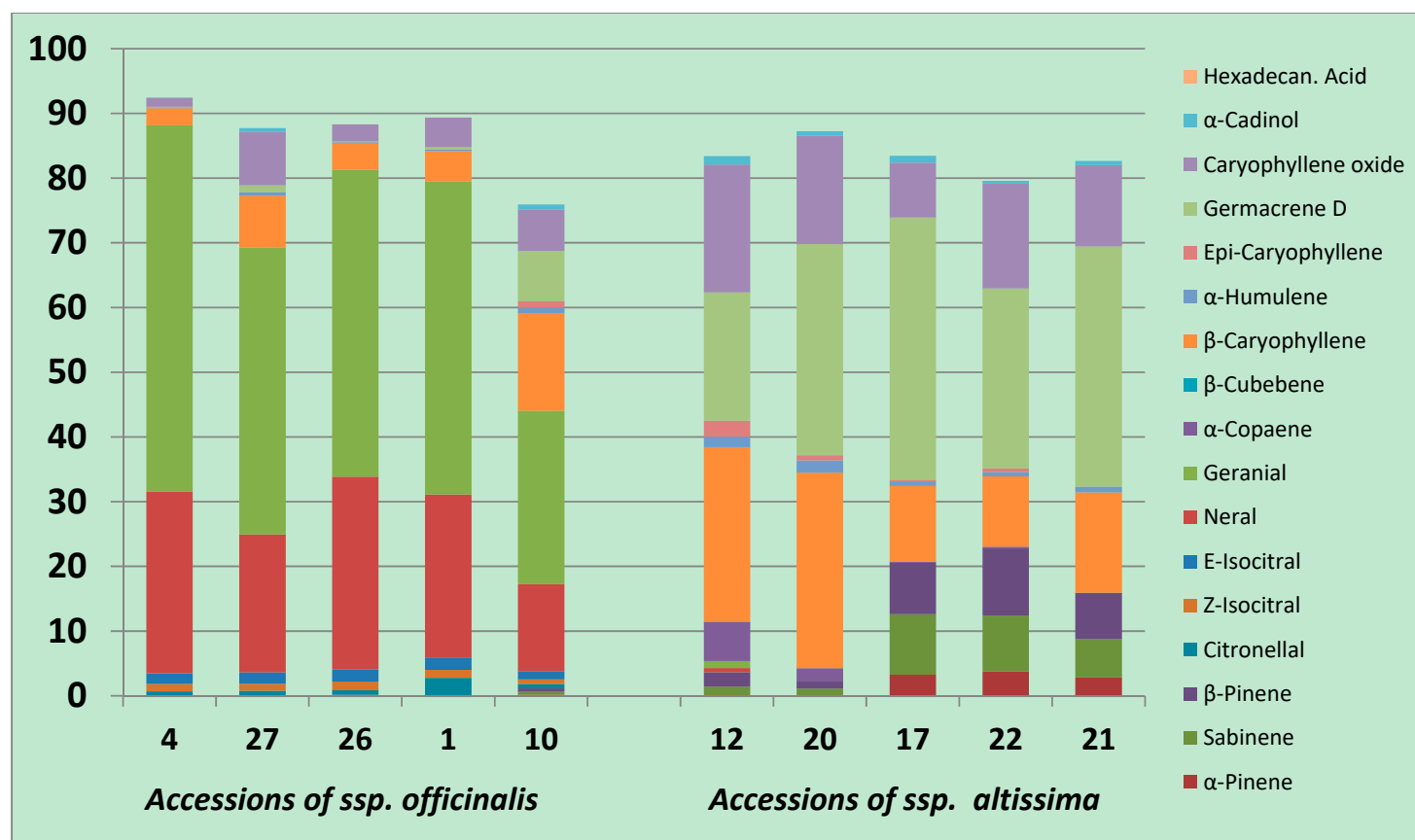


Figure S4: *Melissa officinalis*: composition of the stem essential oils from the 2nd cut

