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Mass Spectral Fragmentation of *Pelargonium graveolens* Essential Oil Using GC–MS Semi-Empirical Calculations and Biological Potential

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Supplementary Materials:

Table S1. The chemical composition of *P. graveolens* essential oil by GC-MS.

peak	R.t*	Name	Retention index (RI)	Area %	Molecular Weight	Molecular formula
1	2.79	Cyclopentane, methyl-	631	1.00	84	C ₆ H ₁₂
2	7.01	α-Pinene	929	1.23	136	C ₁₀ H ₁₆
3	7.85	2H-Pyran, 2-ethenyltetrahydro-2,6,6-trimethyl	972	0.50	154	C ₁₀ H ₁₈ O
4	8.12	á-Pinene	979	0.17	136	C ₁₀ H ₁₆
5	9.05	D-Limonene	1317	0.54	136	C ₁₀ H ₁₆
6	9.28	trans-3-Caren-2-ol	-	0.42	152	C ₁₀ H ₁₆ O
7	10.17	cis-Linalool Oxide	1074	0.38	170	C ₁₀ H ₁₈ O ₂
8	10.58	β-LINALOOL	1099	10.05	154	C ₁₀ H ₁₈ O
9	10.78	Rose oxide	1110	5.77	154	C ₁₀ H ₁₈ O
10	11.14	cis Rose oxide	-	0.79	154	C ₁₀ H ₁₈ O
11	12.23	ISO MENTHONE	1164	4.16	154	C ₁₀ H ₁₈ O
12	12.57	cis-Menthone	1164	10.23	154	C ₁₀ H ₁₈ O
13	13.24	β-CITRONELLOL	-	17.33	156	C ₁₀ H ₂₀ O
14	14.05	Citronellol	1228	11.34	156	C ₁₀ H ₂₀ O
15	14.22	á-Citral	1240	0.59	152	C ₁₀ H ₁₆ O
16	14.94	Geraniol formate	1300	6.87	182	C ₁₁ H ₁₈ O ₂
17	15.72	2,6-Octadiene, 2,6-dimethyl-	978	0.50	138	C ₁₀ H ₁₈
18	15.96	Copaene	1376	0.97	204	C ₁₅ H ₂₄
19	16.34	(-)-β-Bourbonene	1384	2.06	204	C ₁₅ H ₂₄
20	16.86	Nerolidyl acetate	1687	0.64	264	C ₁₇ H ₂₈ O ₂
21	17.49	Caryophyllene	1419	2.30	204	C ₁₅ H ₂₄
22	18.19	(-)-Alloaromadendrene	1440	0.83	204	C ₁₅ H ₂₄
23	19.22	D-Germacrene	1481	1.70	204	C ₁₅ H ₂₄
24	20.05	δ-Cadinene	1524	3.55	204	C ₁₅ H ₂₄
25	20.67	trans-Calamenene	1529	0.74	202	C ₁₅ H ₂₂
26	21.03	Geranyl stearate	2951	0.80	224	C ₁₄ H ₂₄ O ₂
27	21.81	Diepicedrene-1-oxide	1551	0.71	220	C ₁₅ H ₂₄ O
28	23.55	ς-Eudesmol	1631	9.40	222	C ₁₅ H ₂₆ O
29	24.34	Epiglobulol	1585	0.80	222	C ₁₅ H ₂₆ O
30	24.79	Geranyl tiglate	1702	2.80	236	C ₁₅ H ₂₄ O ₂

*R.t, retention time (min).



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