

Phytochemical Constituents and Antiproliferative Activities of Essential Oils from Four Varieties of Malaysian *Zingiber officinale* Roscoe against Human Cervical Cancer Cell Line

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Supplementary material

Table S1 Secondary compounds tentatively identified in different ginger oils using GC-MS. Repeated entries for a given compound correspond to the different ginger varieties.

No	Compound	^a T _R (min)	CASRN	Molecular formula	^b Class	^c Match Factor (Reverse Match Factor)	^d m/z of significant ions (relative ion abundance)	RI _{ref}	^e RI _{cal} (relative percentage abundance, %)			
									BE	CH	SA	BA
1	2-Heptanol	8.7	543-49-7	C ₇ H ₁₆ O	OA	922 (923); 920 (924); 911 (914)	45.1(100), 55.1 (21.9), 83.1 (14.8); 45.1(100), 55.1 (25.8), 83.1 (16.4); 45.1(100), 55.1 (23.4), 83.1 (15.2)	901	901 (0.4 ± 0.065)	8NA	901 (0.1 ± 0.002)	901 (0.1 ± 0.016)
2	Tricyclene	9.5	508-32-7	C ₁₀ H ₁₆	MH	913 (913); 912 (912); 909 (909); 917 (917)	93.1 (100), 91.1 (29.8), 121.1 (24.2); 93.1 (100), 91.1 (29.5), 121.1 (24.6); 93.1 (100), 91.1 (30.9), 121.1 (22.9); 93.1 (100), 91.1 (29.9), 121.1 (24.7)	919	918 (0.3 ± 0.046)	919 (0.2 ± 0.046)	918 (0.2 ± 0.001)	918 (0.3 ± 0.036)
3	Pinene, α-	10.0	80-56-8	C ₁₀ H ₁₆	MH	931 (932); 934 (934); 930 (930); 933 (933)	93.1 (100), 91.1 (43.3), 92.1 (37.5); 93.1 (100), 91.1 (43.3), 92.1 (37.5); 93.1 (100), 91.1 (45.3), 92.1 (37.8); 93.1 (100), 91.1 (42.4), 92.1 (37.4)	931	931 (4.0 ± 0.714)	931 (3.3 ± 0.831)	931 (3.0 ± 0.035)	931 (2.8 ± 0.371)
4	Camphene	10.7	79-92-5	C ₁₀ H ₁₆	MH	958 (967); 959 (966); 958 (965); 959 (967)	93.1 (100), 121.2 (74.9), 79.1 (36.2); 93.1 (100), 121.2 (76.7), 79.1 (35.9); 93.1 (100), 121.1 (72.6), 91.1 (36.2); 93.1 (100), 121.2 (76.8), 79.1 (36.2)	946	946 (9.4 ± 1.708)	946 (7.2 ± 1.748)	945 (7.2 ± 0.101)	946 (10.5 ± 1.452)
5	Sabinene	11.8	3387-41-5	C ₁₀ H ₁₆	MH	914 (929); 922 (928); 907 (914); 901 (909)	93.1 (100), 91.1 (40.2), 77.1 (33.5); 93.1 (100), 91.1 (42.6), 77.1 (33.3); 93.1 (100), 91.1 (44.2), 77.1 (34.7); 93.1 (100), 91.1 (43.0), 77.1 (31.4)	971	970 (0.1 ± 0.022)	971 (0.1 ± 0.027)	971 (0.1 ± 0.001)	971 (0.1 ± 0.013)
6	Pinene, β-	11.9	127-91-3	C ₁₀ H ₁₆	MH	906 (906); 910 (910); 893 (893); 900 (900)	93.1 (100), 69.1 (28.2), 91.1 (27.9); 93.1 (100), 91.1 (27.4), 69.1 (27.2); 93.1 (100), 91.1 (29.6), 69.1 (26.0); 93.1 (100), 69.1 (27.4), 91.1 (27.3)	973	973 (0.8 ± 0.139)	973 (0.7 ± 0.180)	973 (0.4 ± 0.004)	973 (0.3 ± 0.035)
7	Sulcatone	12.5	110-93-0	C ₈ H ₁₄ O	AK	906 (914); 892 (899); 863 (866); 912 (919)	108.1 (100), 69.1 (74.8), 55.1 (69.7); 108.1 (100), 69.1 (73.0), 55.1 (68.1); 108.1 (100), 69.1 (70.5), 55.1 (68.5); 108.1 (100), 69.1 (73.3), 55.1 (67.2)	987	987 (0.3 ± 0.065)	987 (0.1 ± 0.027)	987 (0.1 ± 0.002)	987 (0.5 ± 0.062)

Table S1 (continued)

8	Myrcene, β -	12.7	123-35-3	C ₁₀ H ₁₆	MH	941 (949); 930 (938); 925 (933); 935 (944)	93.1 (100), 69.1 (65.1), 91.1 (23.0); 93.1 (100), 69.1 (64.0), 91.1 (23.0); 93.1 (100), 69.1 (62.9), 91.1 (24.4); 93.1 (100), 69.1 (64.5), 91.1 (22.8)	991	992 (2.2 \pm 0.394)	992 (1.8 \pm 0.483)	991 (1.5 \pm 0.022)	991 (1.5 \pm 0.182)
9	Phellandrene, α -	13.2	99-83-2	C ₁₀ H ₁₆	MH	845 (921); 856 (922); 876 (912); 888 (923)	93.1 (100), 91.1 (55.7), 77.1 (33.4); 93.1 (100), 91.1 (55.1), 77.1 (32.6); 93.1 (100), 91.1 (57.7), 77.1 (34.2); 93.1 (100), 91.1 (55.4), 77.1 (33.1)	1002	1002 (0.6 \pm 0.102)	1002 (0.5 \pm 0.118)	1002 (0.6 \pm 0.009)	1002 (0.6 \pm 0.073)
10	3-Carene	13.5	13466-78-9	C ₁₀ H ₁₆	MH	921 (928); 920 (924); 919 (923); 937 (938)	93.1 (100), 91.1 (46.1), 77.1 (30.6); 93.1 (100), 91.1 (48.1), 77.1 (30.7); 93.1 (100), 91.1 (49.7), 77.1 (35.3); 93.1 (100), 91.1 (49.3), 77.1 (31.9)	1008	1008 (0.1 \pm 0.021)	1008 (0.1 \pm 0.023)	1008 (0.1 \pm 0.032)	1008 (0.06 \pm 0.009)
11	Cymene, p-	14.2	99-87-6	C ₁₀ H ₁₄	MH	884 (888); 940 (945); 874 (876); 890 (891)	119.1 (100), 91.1 (22.3), 134.1 (20.9); 119.1 (100), 134.1 (27.4), 91.1 (18.8); 119.1 (100), 134.1 (28.0), 91.1 (17.7); 119.1 (100), 134.1 (28.0), 91.1 (19.7)	1023	1023 (0.1 \pm 0.025)	1023 (0.1 \pm 0.015)	1023 (0.1 \pm 0.004)	1023 (0.2 \pm 0.025)
12	Phellandrene, β -	14.4	555-10-2	C ₁₀ H ₁₆	MH	867 (904); 857 (884); 901 (904); 883 (895)	93.1 (100), 91.1 (44.1), 77.1 (33.0); 93.1 (100), 91.1 (43.2), 77.1 (32.3); 93.1 (100), 91.1 (43.2), 77.1 (32.3); 93.1 (100), 91.1 (44.7), 77.1 (33.2)	1028	1028 (7.2 \pm 1.217)	1028 (5.0 \pm 1.251)	1028 (7.4 \pm 0.079)	1028 (7.9 \pm 1.012)
13	Eucalyptol	14.5	470-82-6	C ₁₀ H ₁₈ O	MO	940 (940); 931 (931); 917 (917); 934 (934)	81.1 (100), 108.1 (92.7), 111.1 (80.3); 81.1 (100), 108.1 (94.4), 154.2 (80.9); 81.1 (100), 108.1 (97.4), 111.1 (85.6); 81.1 (100), 108.1 (92.8), 154.2 (79.7)	1029	1029 (4.1 \pm 0.675)	1029 (2.4 \pm 0.642)	1028 (2.3 \pm 0.038)	1029 (2.3 \pm 0.314)
14	2-Heptanol, acetate	15.2	5921-82-4	C ₉ H ₁₈ O ₂	AE	926 (927); 887 (892); 932 (932)	87.1 (100), 56.1 (45.9), 98.1 (41.4); 87.1 (100), 56.1 (42.2), 98.1 (40.5); 87.1 (100), 56.1 (41.3), 98.2 (38.5)	1054	1044 (0.1 \pm 0.010)	1044 (0.1 \pm 0.040)	NA	1044 (0.1 \pm 0.013)

Table S1 (continued)

15	Terpinene, γ -	15.8	99-85-4	C ₁₀ H ₁₆	<i>MH</i>	817 (912); 877 (899); 813 (870); 848 (889)	93.1 (100), 91.1 (49.1), 136.2 (35.4); 93.1 (100), 91.1 (53.3), 136.2 (43.0); 93.1 (100), 91.1 (47.6), 136.2 (45.5); 93.1 (100), 91.1 (49.9), 136.2 (36.3)	1057	1057 (0.1 \pm 0.021)	1057 (0.1 \pm 0.021)	1057 (0.1 \pm 0.001)	1057 (0.1 \pm 0.010)
16	Terpinolene	17.2	586-62-9	C ₁₀ H ₁₆	<i>MH</i>	902 (910); 915 (923); 875 (876); 896 (907)	121.1 (100), 93.1 (94.7), 136.2 (87.6); 121.1 (100), 93.1 (92.8), 136.2 (88.2); 121.1 (100), 93.1 (91.8), 136.2 (87.7); 121.1 (100), 93.1 (92.6), 136.2 (87.8)	1085	1086 (0.6 \pm 0.092)	1086 (0.7 \pm 0.331)	1086 (0.4 \pm 0.005)	1086 (0.4 \pm 0.065)
17	2-Nonanone	17.5	821-55-6	C ₉ H ₁₈ O	<i>AK</i>	873 (887); 879 (910); 818 (853); 924 (928)	58.1 (100), 71.1 (26.0), 59.1 (22.8); 58.1 (100), 71.1 (25.7), 57.1 (21.6); 58.1 (100), 71.1 (24.3), 57.1 (23.7); 58.1 (100), 71.1 (26.0), 57.1 (23.2)	1092	1092 (0.3 \pm 0.035)	1092 (0.1 \pm 0.046)	1092 (0.1 \pm 0.002)	1092 (0.5 \pm 0.055)
18	Rosefuran	17.7	15186-51-3	C ₁₀ H ₁₄ O	<i>MO</i>	904 (906); 920 (924); 873 (874); 914 (919)	150.2 (100), 135.1 (89.6), 91.1 (39.7); 150.1 (100), 135.1 (80.9), 91.1 (41.7); 150.1 (100), 135.1 (92.1), 91.1 (41.1); 150.2 (100), 135.1 (93.2), 91.1 (42.5)	1095	1097 (0.3 \pm 0.036)	1097 (0.1 \pm 0.003)	1097 (0.2 \pm 0.008)	1097 (0.1 \pm 0.011)
19	Linalool	17.8	78-70-6	C ₁₀ H ₁₈ O	<i>OM</i>	887 (902); 892 (900); 891 (901); 864 (880)	71.1 (100), 93.1 (90.0), 69.1 (62.5); 71.1 (100), 93.1 (90.4), 69.1 (63.3); 71.1 (100), 93.1 (94.2), 69.1 (58.1); 71.1 (100), 93.1 (88.1), 69.1 (60.4)	1100	1100 (0.7 \pm 0.090)	1100 (1.0 \pm 0.507)	1100 (0.6 \pm 0.008)	1100 (1.2 \pm 0.125)
20	2-Nonanol	17.9	628-99-9	C ₉ H ₂₀ O	<i>OA</i>	866 (920)	45.1 (100), 69.1 (35.2), 55.1 (19.1)	1100	1101 (0.6 \pm 0.092)	NA	NA	NA
21	1,3,7-Nonatriene, 4,8-dimethyl-	18.7	19945-61-0	C ₁₁ H ₁₈	<i>AH</i>	893 (912); 895 (912); 892 (900)	69.1 (100), 81.1 (19.0), 79.1 (16.5); 69.1 (100), 81.1 (18.5), 79.1 (16.3); 69.1 (100), 81.1 (20.7), 79.0 (20.2)	1118	1117 (0.1 \pm 0.013)	1117 (0.1 \pm 0.058)	1117 (0.1 \pm 0.005)	NA
22	Camphor	19.8	76-22-2	C ₁₀ H ₁₆ O	<i>MK</i>	941 (941); 951 (958)	95.1 (100), 81.1 (66.7), 108.1 (47.4); 95.1 (100), 81.1 (65.1), 108.1 (40.9)	1142	1141 (0.1 \pm 0.008)	NA	NA	1141 (0.1 \pm 0.012)

Table S1 (continued)

23	Citronellal	20.4	2385-77-5	C ₁₀ H ₁₈ O	MA	918 (918); 913 (913); 922 (923); 890 (890)	69.1 (100), 95.1 (77.4), 55.1 (45.9); 69.1 (100), 95.1 (86.2), 55.1 (46.9); 69.1 (100), 95.1 (86.8), 55.1 (46.7); 95.1 (100), 69.1 (82.7), 55.1 (40.6)	1152	1154 (0.8 ± 0.081)	1153 (0.3 ± 0.140)	1153 (0.5 ± 0.003)	1154 (0.3 ± 0.040)
24	Borneol	20.8	507-70-0	C ₁₀ H ₁₈ O	OM	923 (923); 917 (917); 910 (910); 940 (940)	95.1 (100), 110.2 (20.6), 93.1 (9.1); 95.1 (100), 110.1 (20.7), 93.1 (9.0); 95.1 (100), 110.1 (20.2), 67.1 (9.8); 95.1 (100), 110.2 (21.1), 7.1 (9.6)	1163	1163 (0.8 ± 0.094)	1163 (0.6 ± 0.282)	1163 (0.7 ± 0.012)	1163 (2.7 ± 0.302)
25	Iso-citral	20.9	72203-97-5	C ₁₀ H ₁₆ O	MA	986 (907); 925 (926); 875 (876); 889 (890)	109.1 (100), 81.1 (96.6), 67.1 (94.3); 109.1 (100), 81.1 (93.2), 94.1 (90.6); 109.1 (100), 81.1 (96.6), 67.1 (93.3); 109.1 (100), 94.1 (93.6), 81.1 (92.6)	1160	1165 (0.5 ± 0.054)	1165 (0.4 ± 0.244)	1165 (0.5 ± 0.009)	1165 (0.5 ± 0.059)
26	4-Terpineol	21.4	562-74-3	C ₁₀ H ₁₈ O	OM	803 (834); 852 (876); 800 (825); 801 (836)	71.1 (100), 95.1 (70.1), 111.1 (65.6); 71.1 (100), 93.1 (70.7), 111.1 (69.9); 71.1 (100), 111.1 (69.3), 93.1 (65.6); 71.1 (100), 95.1 (92.1), 111.1 (66.0)	1175	1175 (0.1 ± 0.015)	1175 (0.1 ± 0.039)	1175 (0.2 ± 0.09)	1175 (0.3 ± 0.031)
27	Terpineol, α-	22.1	98-55-5	C ₁₀ H ₁₈ O	OM	907 (907); 900 (900); 882 (882); 899 (899)	59.1 (100), 93.1 (82.2), 121.1 (75.7); 59.1 (100), 93.1 (83.8), 121.1 (78.0); 59.1 (100), 93.1 (88.3), 121.1 (85.2); 59.1 (100), 93.1 (81.7), 121.1 (76.1)	1189	1189 (0.9 ± 0.114)	1189 (0.8 ± 0.242)	1189 (0.6 ± 0.006)	1189 (0.6 ± 0.070)
28	Citral, β-	24.6	106-26-3	C ₁₀ H ₁₆ O	MA	929 (929); 936 (936); 926 (926); 936 (937)	69.1 (100), 94.1 (37.0), 109.1 (36.2); 69.1 (100), 94.1 (36.6), 109.1 (35.4); 69.1 (100), 109.1 (40.0), 94.1 (37.8); 69.1 (100), 94.1 (36.9), 109.1 (35.9)	1244	1245 (8.0 ± 0.981)	1244 (5.6 ± 0.528)	1244 (6.8 ± 0.030)	1244 (8.1 ± 0.922)
29	Geraniol	25.3	106-24-1	C ₁₀ H ₁₈ O	OM	930 (930); 929 (929); 924 (924); 937 (937)	69.1 (100), 68.1 (20.0), 93.1 (17.3); 69.1 (100), 68.1 (19.9), 93.1 (18.2); 69.1 (100), 68.1 (20.0), 93.1 (19.2); 69.1 (100), 68.1 (19.9), 93.1 (14.6)	1259	1259 (2.6 ± 0.319)	1260 (5.0 ± 0.568)	1258 (1.8 ± 0.008)	1259 (4.2 ± 0.428)

Table S1 (continued)

31	Bornyl acetate	26.5	5655-61-8	C ₁₂ H ₂₀ O ₂	MAc	916 (917); 912 (912); 910 (910); 917 (917)	95.1 (100), 93.1 (48.4), 121.1 (43.0); 95.1 (100), 93.1 (46.6), 121.1 (45.9); 95.1 (100), 93.1 (54.5), 136.2 (43.2); 95.1 (100), 93.1 (46.5), 121.1 (45.6)	1285	1286 (0.1 ± 0.016)	1286 (0.3 ± 0.033)	1286 (0.1 ± 0.001)	1286 (0.6 ± 0.150)
32	2-Undecanone	26.9	112-12-9	C ₁₁ H ₂₂ O	AK	938 (949); 910 (922); 913 (923); 933 (941)	58.1 (100), 71.1 (37.9), 59.1 (30.0); 58.1 (100), 71.1 (38.2), 59.1 (29.8); 58.1 (100), 71.1 (39.3), 59.1 (30.0); 58.1 (100), 71.1 (37.8), 59.1 (29.8)	1295	1295 (0.7 ± 0.117)	1295 (0.2 ± 0.029)	1295 (0.5 ± 0.002)	1295 (0.6 ± 0.178)
33	2-Undecanol	27.2	1653-30-1	C ₁₁ H ₂₄ O	OA	922 (947); 892 (930); 902 (918); 874 (913)	45.1 (100), 55.1 (23.6), 83.1 (22.5); 45.1 (100), 55.1 (27.0), 83.1 (23.5); 45.1 (100), 83.1 (26.2), 83.1 (21.9); 45.1 (100), 55.1 (27.3), 83.1 (26.1)	1301	1302 (0.2 ± 0.032)	1302 (0.1 ± 0.011)	1302 (0.1 ± 0.001)	1302 (0.1 ± 0.020)
34	Elemene, δ-	28.7	20307-84-0	C ₁₅ H ₂₄	SH	897 (900); 915 (915)	121.1 (100), 93.1 (65.9), 136.2 (61.5); 121.1 (100), 93.1 (64.7), 136.1 (53.7)	1337	NA	1337 (0.3 ± 0.248)	1337 (0.1 ± 0.001)	NA
35	Citronellyl acetate	29.5	150-84-5	C ₁₂ H ₂₂ O ₂	MAc	806 (819); 903 (904); 905 (905); 901 (902)	95.1 (100), 81.1 (97.5), 69.1 (97.0); 81.1 (100), 95.1 (99.7), 69.1 (94.2); 95.1 (100), 81.1 (93.2), 69.1 (86.8); 81.1 (100), 95.1 (98.9), 69.1 (94.0)	1355	1355 (0.1 ± 0.038)	1355 (0.7 ± 0.217)	1355 (0.1 ± 0.001)	1355 (0.4 ± 0.090)
36	Cyclosativene	29.9	22469-52-9	C ₁₅ H ₂₄	SH	897 (898); 884 (885); 851 (851); 918 (920)	105.1 (100), 161.2 (97.1), 204.3 (79.8); 105.1 (100), 161.2 (83.9), 119.1 (76.5); 161.2 (100), 105.1 (83.5), 119.1 (68.8); 105.1 (100), 161.2 (95.6), 119.1 (82.0)	1362	1363 (0.1 ± 0.024)	1363 (0.1 ± 0.038)	1363 (0.1 ± 0.009)	1363 (0.1 ± 0.023)
37	Copaene	30.4	3856-25-5	C ₁₅ H ₂₄	SH	896 (896); 891 (891); 874 (874); 866 (866)	161.2 (100), 119.1 (95.3), 105.1 (86.3); 161.2 (100), 119.1 (95.7), 105.1 (85.6); 161.2 (100), 119.1 (95.3), 105.1 (86.3); 161.2 (100), 119.1 (93.4), 105.1 (83.2)	1374	1374 (0.2 ± 0.060)	1374 (0.3 ± 0.027)	1374 (0.3 ± 0.001)	1374 (0.2 ± 0.038)
38	Geranyl acetate	30.8	105-87-3	C ₁₂ H ₂₀ O ₂	MAc	893 (905); 934 (937); 881 (899); 941 (942)	69.1 (100), 93.1 (46.9), 68.1 (41.6); 69.1 (100), 68.1 (38.8), 93.1 (34.3); 69.1 (100), 93.1 (52.4), 68.1 (37.7); 69.1 (100), 68.1 (38.6), 93.1 (34.4)	1385	1385 (0.2 ± 0.053)	1388 (6.4 ± 0.533)	1385 (0.2 ± 0.001)	1386 (2.3 ± 0.582)

Table S1 (continued)

39	Elemene, β -	31.1	515-13-9	C ₁₅ H ₂₄	SH	883 (900); 877 (877); 877 (892); 885 (899)	93.1 (100), 81.1 (87.6), 67.1 (64.6); 93.1 (100), 81.1 (87.6), 67.1 (64.6); 93.1 (100), 81.1 (86.4), 107.1 (68.4); 93.1 (100), 81.1 (83.4), 107.1 (62.6)	1391	1391 (0.5 \pm 0.152)	1391 (0.7 \pm 0.053)	1391 (0.7 \pm 0.018)	1391 (0.3 \pm 0.079)
40	Sesquithujene	31.7	58319-06-5	C ₁₅ H ₂₄	SH	897 (905); 905 (957); 899 (953); 911 (968)	93.1 (100), 119.1 (91.5), 91.1 (46.6); 119.1 (100), 93.1 (86.0), 91.1 (40.4); 119.1 (100), 93.1 (95.5), 91.1 (46.1); 119.1 (100), 93.1 (90.6), 91.1 (39.9)	1405	1406 (0.1 \pm 0.014)	1406 (0.1 \pm 0.009)	1406 (0.1 \pm 0.001)	1406 (0.1 \pm 0.027)
41	Caryophyllene	32.2	87-44-5	C ₁₅ H ₂₄	SH	846 (846); 844 (844); 863 (863); 822 (824)	91.1 (100), 161.1 (94.4), 120.1 (76.6); 161.1 (100), 91.1 (90.0), 120.1 (78.4); 161.2 (100), 91.1 (76.4), 120.1 (76.0); 91.1 (100), 107.1 (72.9), 79.0 (61.3)	1417	1417 (0.1 \pm 0.039)	1417 (0.1 \pm 0.015)	1417 (0.1 \pm 0.001)	1417 (0.1 \pm 0.035)
42	Elemene, γ -	32.8	29873-99-2	C ₁₅ H ₂₄	SH	919 (940); 923 (945); 917 (917); 846 (882)	121.1 (100), 93.1 (62.1), 107.1 (37.8); 121.1 (100), 93.1 (61.9), 107.1 (44.2); 121.1 (100), 93.1 (62.6), 107.1 (42.7); 121.1 (100), 93.1 (69.5), 107.1 (55.6)	1433	1433 (0.4 \pm 0.090)	1433 (0.4 \pm 0.041)	1433 (0.5 \pm 0.009)	1433 (0.1 \pm 0.011)
43	Germacrene D	34.7	23986-74-5	C ₁₅ H ₂₄	SH	912 (933); 919 (936); 916 (934); 863 (891)	161.2 (100), 105.1 (54.1), 91.1 (47.0); 161.2 (100), 105.1 (54.5), 91.1 (46.5); 161.2 (100), 105.1 (54.9), 91.1 (48.1); 161.2 (100), 119.1 (86.4), 105.1 (72.7)	1480	1480 (0.9 \pm 0.153)	1480 (1.2 \pm 0.496)	1480 (1.5 \pm 0.023)	1480 (0.3 \pm 0.043)
44	Curcumene, α -	34.9	644-30-4	C ₁₅ H ₂₂	SH	917 (936); 909 (937); 908 (932); 932 (940)	119.1 (100), 132.1 (87.6), 105.1 (52.5); 119.1 (100), 132.1 (86.7), 105.1 (53.1); 119.1 (100), 132.1 (87.5), 105.1 (53.9); 119.1 (100), 132.1 (88.8), 105.1 (50.3)	1484	1484 (2.6 \pm 0.395)	1483 (2.2 \pm 0.222)	1484 (3.6 \pm 0.045)	1484 (4.5 \pm 0.850)
45	Eudesmene, β -	35.2	17066-67-0	C ₁₅ H ₂₄	SH	926 (950); 926 (950); 931 (931)	161.2 (100), 189.2 (68.8), 105.1 (67.4); 161.2 (100), 189.2 (68.6), 105.1 (67.6); 161.2 (100), 189.2 (72.2), 133.1 (68.8)	1492	1492 (0.6 \pm 0.091)	1492 (0.7 \pm 0.065)	1492 (0.9 \pm 0.131)	NA
46	Zingiberene	35.5	495-60-3	C ₁₅ H ₂₄	SH	861 (886); 902 (955); 896 (951); 898 (950)	119.1 (100), 93.1 (82.9), 91.1 (46.8); 119.1 (100), 93.1 (84.4), 91.1 (42.8); 119.1 (100), 93.1 (82.9), 91.1 (46.7); 119.1 (100), 93.1 (84.3), 91.1 (43.7)	1499	1499 (7.9 \pm 1.132)	1498 (12.1 \pm 1.003)	1497 (14.0 \pm 1.288)	1499 (10.8 \pm 1.863)

Table S1 (continued)

47	Bisabolene, β -	36.0	495-61-4	C ₁₅ H ₂₄	SH	890 (899); 942 (948); 936 (942); 886 (886)	93.1 (100), 69.1 (56.3), 107.1 (48.1); 93.1 (100), 107.1 (52.6), 119.1 (47.2); 93.1 (100), 107.1 (54.9), 91.1 (46.5); 93.1 (100), 69.1 (66.1), 107.1 (44.0)	1510	1510 (4.6 \pm 0.696)	1510 (7.4 \pm 0.598)	1510 (8.4 \pm 0.145)	1510 (4.6 \pm 0.909)
48	Sesquiphellandrene , β -	36.6	20307-83-9	C ₁₅ H ₂₄	SH	906 (917); 936 (925); 899 (910); 912 (936)	69.1 (100), 93.1 (68.4), 91.1 (64.8); 69.1 (100), 93.1 (68.0), 91.1 (61.1); 69.1 (100), 93.1 (68.0), 91.1 (61.1); 69.1 (100), 93.1 (67.6), 91.1 (60.9)	1525	1525 (3.2 \pm 0.511)	1526 (4.6 \pm 0.468)	1526 (5.2 \pm 0.065)	1526 (4.5 \pm 0.967)
49	Bisabolene, γ -	36.8	53585-13-0	C ₁₅ H ₂₄	SH	879 (930); 876 (912); 867 (900); 874 (907)	93.1 (100), 107.1 (99.5), 119.1 (48.2); 93.1 (100), 107.1 (94.6), 119.1 (49.4); 93.1 (100), 107.1 (90.6), 119.1 (52.0); 93.1 (100), 107.1 (94.6), 119.1 (44.8)	1533	1532 (0.1 \pm 0.022)	1532 (0.2 \pm 0.027)	1533 (0.2 \pm 0.008)	1533 (0.1 \pm 0.023)
50	Elemol	37.5	21657-90-9	C ₁₅ H ₂₆ O	OS	926 (929); 926 (929); 941 (946); 918 (921)	93.1 (100), 59.1 (98.7), 161.2 (80.1); 93.1 (100), 59.1 (96.9), 161.2 (81.9); 93.1 (100), 59.1 (91.3), 161.2 (85.4); 93.1 (100), 59.1 (97.7), 161.2 (80.8)	1549	1549 (0.9 \pm 0.105)	1549 (1.2 \pm 0.122)	1549 (0.7 \pm 0.007)	1549 (0.3 \pm 0.077)
51	Nerolidol	38.1	40716-66-3	C ₁₅ H ₂₆ O	OS	928 (932); 928 (932); 922 (925); 902 (909)	69.1 (100), 93.1 (80.7), 107.1 (47.3); 69.1 (100), 93.1 (81.5), 107.1 (47.7); 69.1 (100), 93.1 (86.3), 107.1 (49.4); 69.1 (100), 93.1 (81.9), 107.1 (47.2)	1564	1565 (0.8 \pm 0.251)	1565 (0.8 \pm 0.062)	1564 (0.7 \pm 0.033)	1564 (0.2 \pm 0.023)
52	Sesquisabinene hydrate	39.0	58319-05-4	C ₁₅ H ₂₆ O	OS	891 (897); 890 (896); 879 (885); 886 (889)	69.1 (100), 93.1 (92.8), 119.1 (89.8); 69.1 (100), 93.1 (91.9), 119.1 (89.6); 93.1 (100), 69.1 (99.4), 119.1 (93.8); 69.1 (100), 93.1 (89.8), 119.1 (89.8)	1590	1589 (0.4 \pm 0.061)	1589 (0.3 \pm 0.048)	1589 (0.3 \pm 0.022)	1590 (0.4 \pm 0.092)
53	Eudesmol, γ -	40.1	1209-71-8	C ₁₅ H ₂₆ O	OS	880 (894); 881 (893); 858 (866); 899 (907)	161.2 (100), 189.2 (81.2), 81.1 (65.7); 161.2 (100), 189.2 (80.8), 81.1 (65.1); 161.2 (100), 189.2 (80.8), 81.1 (65.1); 189.2 (100), 161.2 (83.0), 133.1 (55.5)	1620	1618 (0.4 \pm 0.074)	1618 (0.3 \pm 0.008)	1618 (0.3 \pm 0.035)	1618 (0.1 \pm 0.032)

Table S1 (continued)

54	Muurolol, T-	41.0	19912-62-0	C ₁₅ H ₂₆ O	OS	820 (877); 822 (884); 803 (859)	161.2 (100), 95.1 (61.0), 105.1 (47.5); 161.2 (100), 95.1 (58.6), 105.1 (46.1); 161.2 (100), 95.1 (53.8), 204.2 (50.7)	1641	1641 (0.3 ± 0.040)	1641 (0.2 ± 0.034)	1641 (0.2 ± 0.029)	NA
55	Cubenol	41.1	21284-22-0	C ₁₅ H ₂₆ O	OS	810 (868); 834 (890); 813 (866)	161.2 (100), 119.1 (96.4), 95.1 (75.2); 161.2 (100), 119.1 (98.1), 95.1 (70.6); 161.1 (100), 119.1 (94.0), 105.0 (66.1)	1646	1646 (0.1 ± 0.040)	1646 (0.1 ± 0.019)	1646 (0.1 ± 0.006)	NA
56	Eudesmol, β-	41.2	473-15-4	C ₁₅ H ₂₆ O	OS	907 (918); 905 (914); 887 (895); 846 (869)	59.1 (100), 149.2 (85.2), 164.2 (43.1); 59.1 (100), 149.2 (86.6), 164.2 (44.8); 59.1 (100), 149.2 (99.1), 164.2 (50.4); 59.1 (100), 149.2 (86.1), 119.1 (54.0)	1649	1649 (0.8 ± 0.128)	1649 (0.6 ± 0.017)	1649 (0.6 ± 0.005)	1649 (0.4 ± 0.085)
57	Farnesol	43.9	106-28-5	C ₁₅ H ₂₆ O	OS	855 (889)	69.1 (100), 81.1 (33.2), 93.1 (29.8)	1722	NA	1722 (0.1 ± 0.023)	NA	NA
58	Farnesal	44.6	502-67-0	C ₁₅ H ₂₄ O	SA	905 (912); 903 (909); 892 (894); 890 (929)	69.1 (100), 84.1 (55.8), 81.1 (24.7); 69.1 (100), 84.1 (54.6), 81.1 (24.3); 69.1 (100), 84.1 (54.9), 81.1 (22.8); 69.1 (100), 84.1 (56.4), 81.1 (24.1)	1740	1742 (0.2 ± 0.049)	1742 (0.1 ± 0.031)	1742 (0.1 ± 0.007)	1742 (0.1 ± 0.027)
Total identified									82.6	83.8	84.6	87.4

^aRetention time of eluted compounds.

^bClass of chemical compounds: *MH* monoterpenic hydrocarbon, *MO* monoterpenic oxide, *MA* monoterpenic aldehyde, *OM* monoterpenic alcohol, *MK* monoterpenic ketone, *MAc* monoterpenic acetate, *SH* sesquiterpenic hydrocarbon, *SA* sesquiterpenic aldehyde, *OS* sesquiterpenic alcohol, *AH* acyclic hydrocarbon, *AK* acyclic ketone, *AE* acyclic ester, *OA* acyclic alcohol.

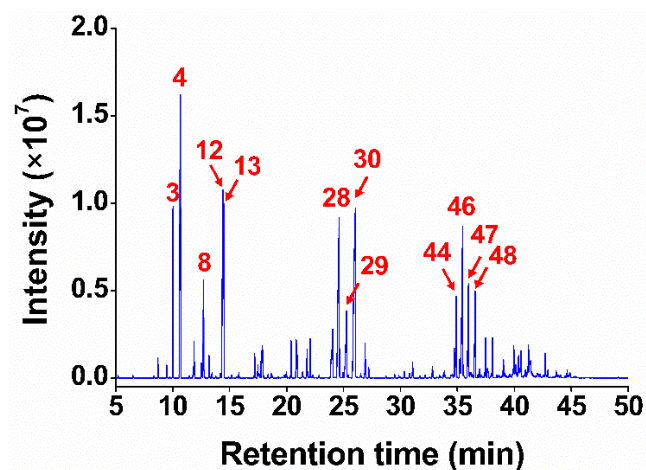
^cMatching scores of compounds reported ≥80% based on mass spectra in NIST library database and in the order of Bentong (BE), Cameron Highlands (CH), Sabah (SA) and Bara (BA) gingers.

^dFragmentation patterns reported in order of BE, CH, SA and BA.

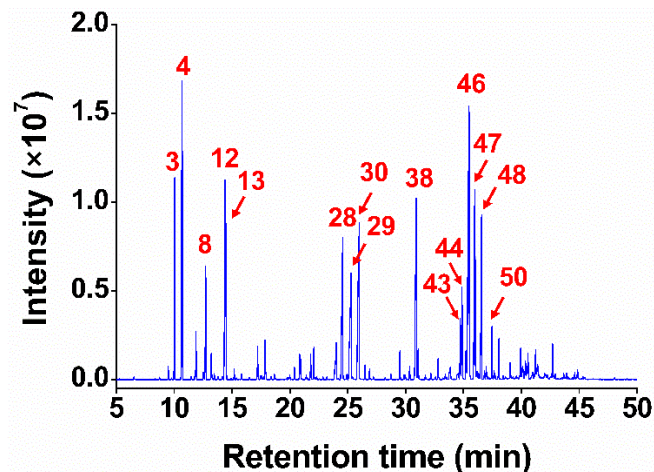
^eRetention index (RI) values calculated using Van Den Dool and Kratz equation with the reference to RI values from NIST WebBook and Adams (2007) within the range of ±10.

^fRelative percentage abundance calculated on the basis of TIC (Total Ion Chromatogram) area as the percentage of total TIC area.

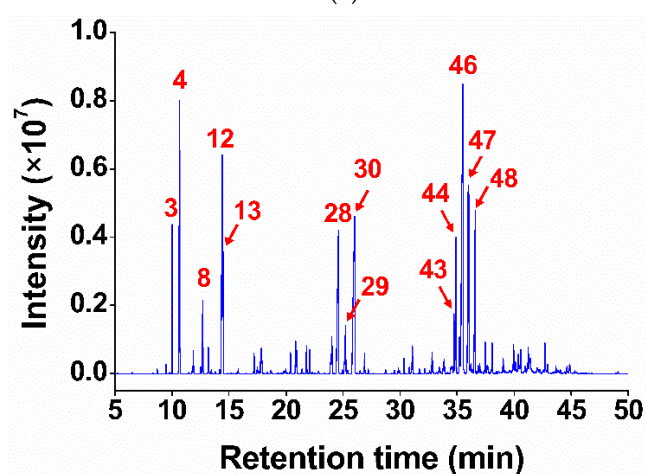
^gNA: compound not available.



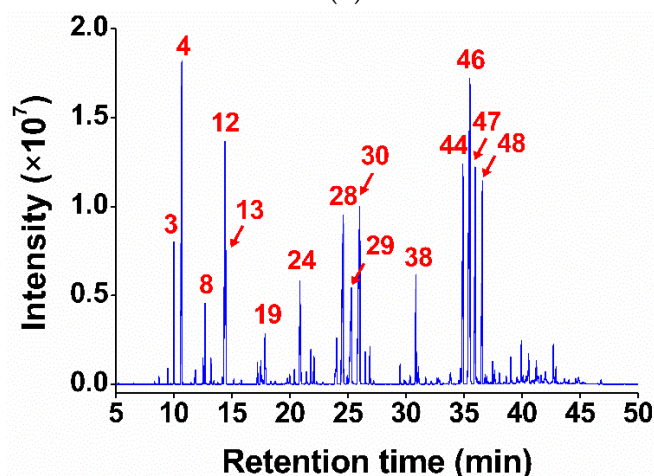
(a)



(b)



(c)



(d)

Figure S1. Total ion chromatograms (TICs) of the volatile profile of *Z. officinale* essential oil varieties. (a) Bentong, BE; (b) Cameron Highlands, CH; (c) Sabah, SA; and (d) Bara, BA. The peak numbering refers to Table S1.