

Supporting Information

Chemical Compositions and Antioxidant Activities of Indonesian Citrus Essential Oils and Their Elucidation Using Principal Component Analysis

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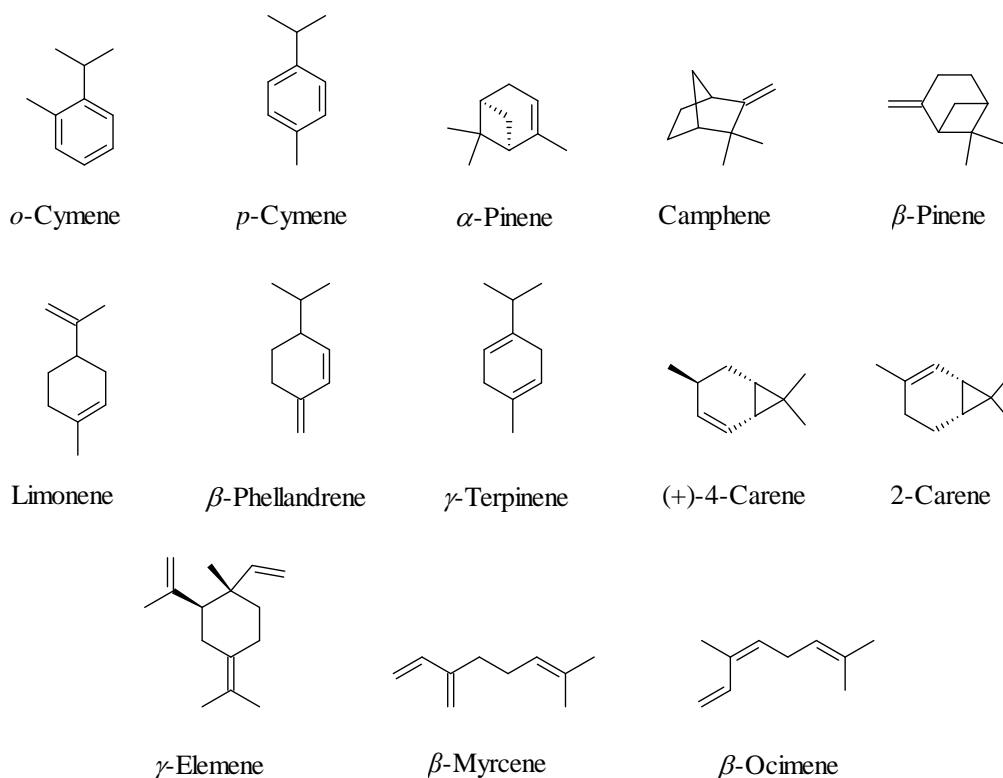
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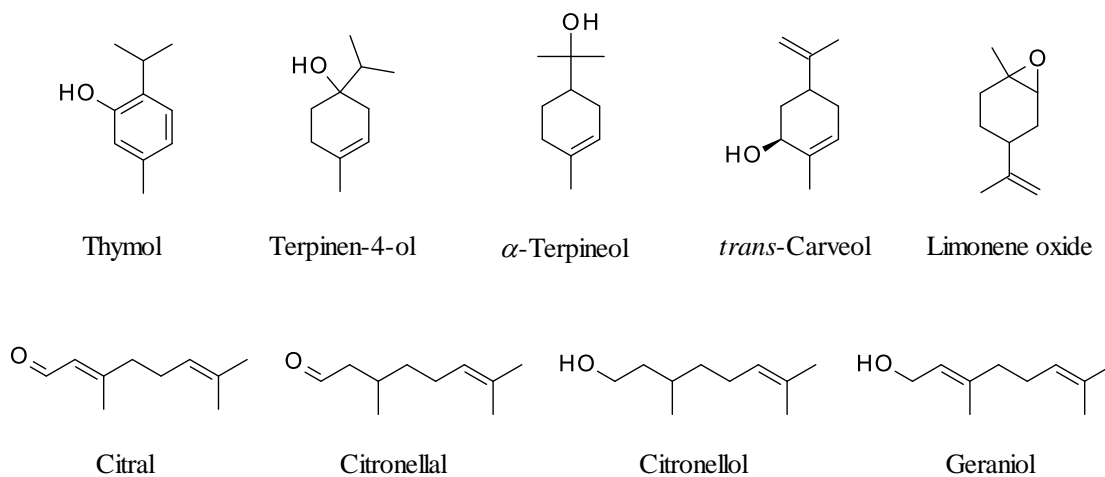
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Figure S1.	Chemical structures of secondary metabolites in essential oils (EOs) of five Indonesian-grown <i>Citrus</i>	2
Figure S2.	Percentage of free-radical scavenging activities of ascorbic acid and five Indonesian-grown <i>Citrus</i>	3
Figure S3.	Score plots on the coordinate systems of all PC combinations. (a) PC1 and PC2, (b) PC1 and PC3, and (c) PC1 and PC4.	3
Table S1.	A matrix containing five rows of <i>Citrus</i> species and twenty-five columns of secondary metabolites.....	4
Table S2.	Representation quality of every descriptor on each PC.	5
Table S3.	DPPH free radical scavenging activities and IC ₅₀ of <i>Citrus</i> EOs.	6

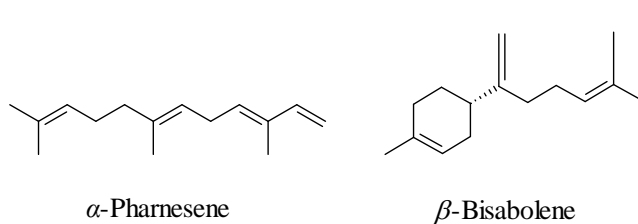
Monoterpenes



Monoterpenoids



Sesquiterpenes



Sesquiterpenoid

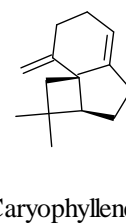


Figure S1. Chemical structures of secondary metabolites in essential oils (EOs) of five Indonesian-grown *Citrus*. These *Citrus* are *C. nobilis*, *C. limon*, *C. aurantifolia*, *C. amblycarpa*, and *Citrus spp.* Some secondary metabolites may be absent in a particular EO (see Table 2 in main text).

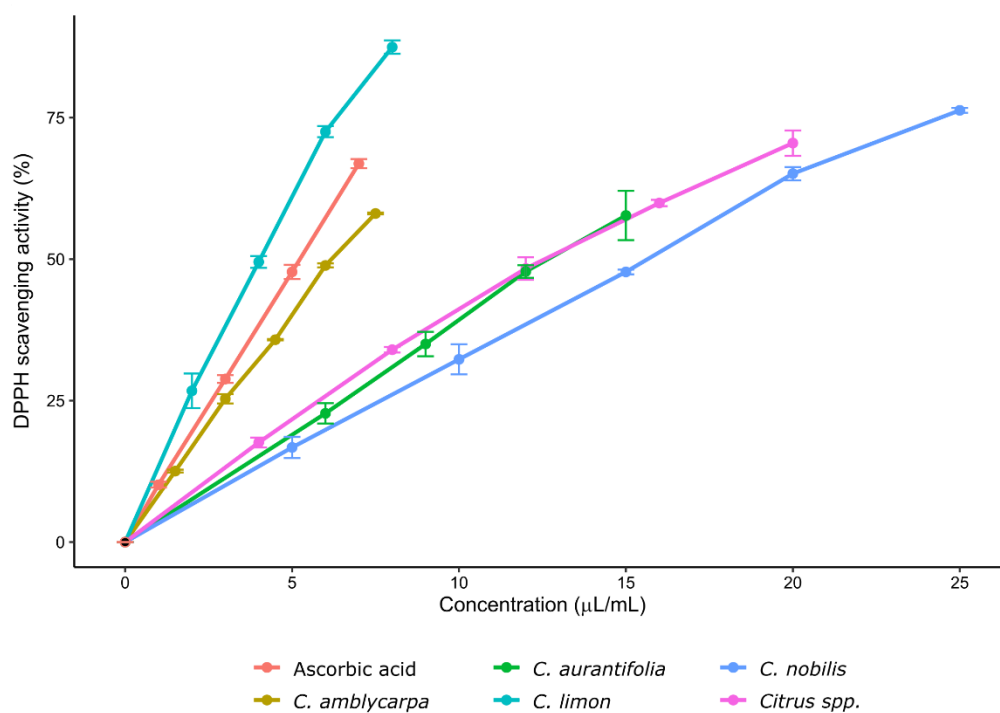


Figure S2. Percentage of free-radical scavenging activities of ascorbic acid and five Indonesian-grown *Citrus*.

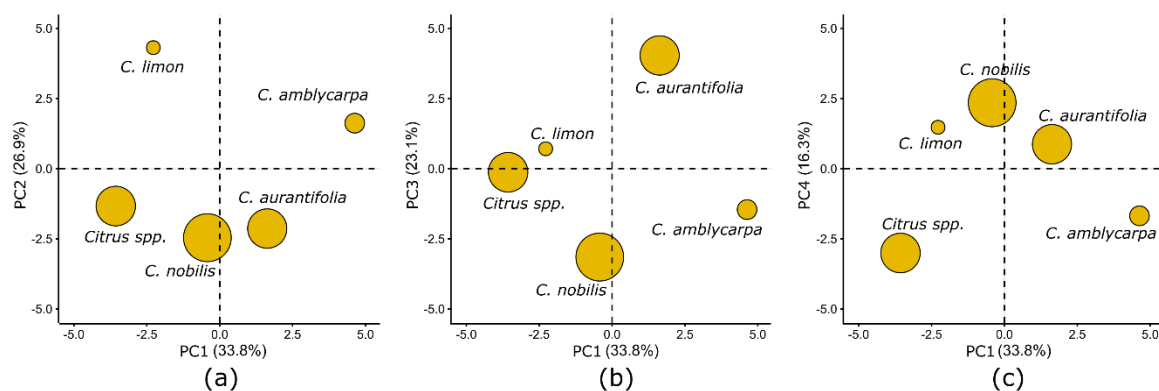


Figure S3. Score plots on the coordinate systems of all PC combinations. (a) PC1 and PC2, (b) PC1 and PC3, and (c) PC1 and PC4.

Table S1. A matrix containing five rows of *Citrus* species and twenty-five columns of secondary metabolites. The five *Citrus* species represent essential oils, whereas the secondary metabolites are descriptors. The values in the matrix are the percent area of secondary metabolites determined by GC-MS.

[illegible]

Table S2. Representation quality of every descriptor on each PC.

	Representation quality (%)			
	PC1	PC2	PC3	PC4
<i>α</i> -Pinene	31	10	58	1
Camphene	88	1	3	8
<i>β</i> -Myrcene	6	30	51	14
<i>β</i> -Pinene	60	0	40	0
<i>D</i> -Limonene	78	0	5	18
<i>β</i> -Phellandrene	77	2	22	0
<i>o</i> -Cymene	13	63	8	17
<i>β</i> -Ocimene	8	73	9	10
<i>γ</i> -Terpinene	2	94	2	3
(+)-4-Carene	8	17	71	5
Terpinen-4-ol	72	10	9	9
<i>α</i> -Terpineol	56	8	2	34
Citral	34	11	1	53
2-Carene	58	33	2	8
Caryophyllene	8	17	71	5
<i>γ</i> -Elemene	8	17	71	5
<i>β</i> -Bisabolene	88	1	2	9
Citronellal	1	23	43	34
Citronellol	65	6	18	11
<i>trans</i> -Carveol	1	23	43	34
Geraniol	1	23	43	34
Thymol	15	69	2	13
<i>p</i> -Cymene	15	69	2	13
<i>α</i> -Pharnesene	15	69	2	13
Limonene oxide	38	7	0	56

Table S3. DPPH free radical scavenging activities and IC₅₀ of *Citrus* EOs.

Concentration ($\mu\text{L/mL}$)	Absorbance		DPPH Scavenging Activity (%)		IC ₅₀ ($\mu\text{L/mL}$)	
	I	II	I	II	I	II
Ascorbic Acid						
0.0	0.766	0.771	0.00	0.00		
1.0	0.691	0.69	9.79	10.38		
3.0	0.549	0.545	28.33	28.79	5.29	5.26
5.0	0.407	0.396	46.87	47.21		
7.0	0.258	0.251	66.32	66.54		
<i>C. limon</i>						
0.0	0.838	0.855	0.00	0.00		
2.0	0.632	0.608	24.58	28.89		
4.0	0.417	0.438	50.24	48.77	4.30	4.20
6.0	0.236	0.229	71.84	73.22		
8.0	0.112	0.100	86.63	88.30		
<i>C. amblycarpa</i>						
0.0	0.873	0.849	0.00	0.00		
1.5	0.765	0.741	12.37	12.72		
3.0	0.647	0.639	25.89	24.73		
4.5	0.56	0.546	35.85	35.69	6.27	6.33
6.0	0.444	0.436	49.14	48.65		
7.5	0.365	0.357	58.19	57.95		
<i>C. aurantifolia</i>						
0.0	0.928	0.908	0.00	0.00		
6.0	0.705	0.713	24.03	23.17		
9.0	0.589	0.604	36.53	34.91	13.0	12.4
12.0	0.477	0.481	48.60	48.17		
15.0	0.421	0.356	54.63	61.64		
<i>Citrus spp.</i>						
0.0	0.835	0.824	0.00	0.00		
4.0	0.683	0.684	18.20	16.99		
8.0	0.554	0.541	33.65	34.34		
12.0	0.443	0.414	46.95	49.76	13.26	13.32
16.0	0.338	0.327	59.52	60.32		
20.0	0.233	0.256	72.10	68.93		
<i>C. nobilis</i>						
0.0	0.714	0.687	0.00	0.00		
5.0	0.604	0.563	18.05	18.05		
10.0	0.470	0.478	30.42	30.42		
15.0	0.371	0.361	47.45	47.45	15.80	15.85
20.0	0.255	0.234	65.94	65.94		
25.0	0.167	0.165	75.98	75.98		

