

Comparative Virucidal Activities of Essential Oils and Alcohol-Based Solutions against Enveloped Virus Surrogates: In Vitro and In Silico Analyses

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Table S1. AutoDock Vina binding energies values of compounds identified in the EO blend for target proteins.

Type	Compound	DENV-2		CHKV
		E	prM/M	E1-E2-E3
Sesquiterpene hydrocarbons	δ-Cadinene	-8.61 ± 0.8	-5.47 ± 0.1	-6.25 ± 0.1
	α-Guaiene	-8.55 ± 1.0	-5.29 ± 0.1	-6.38 ± 0.2
	γ-Cadinene	-8.22 ± 1.0	-5.26 ± 0.2	-6.22 ± 0.1
	α-Bulnesene	-8.12 ± 0.9	-5.37 ± 0.2	-6.26 ± 0.2
	Germacrene D	-7.03 ± 1.1	-5.40 ± 0.1	-6.25 ± 0.2
	β-Elemene	-6.49 ± 0.9	-4.85 ± 0.5	-5.92 ± 0.2
	<i>trans</i> -β-Caryophyllene	-6.48 ± 0.5	-5.36 ± 0.2	-6.32 ± 0.1
	α-Muurolene	-5.91 ± 0.5	-5.26 ± 0.3	-6.18 ± 0.2
	γ-Muurolene	-5.91 ± 0.3	-5.26 ± 0.3	-6.18 ± 0.2
	α-Humulene	-5.90 ± 0.5	-5.29 ± 0.3	-6.37 ± 0.3
	<i>epi</i> -α-Muurolol	-8.10 ± 1.0	-5.42 ± 0.1	-6.37 ± 0.2
	Farnesol *	-6.57 ± 0.6	-5.33 ± 0.2	-6.01 ± 0.2
	α-Cadinol *	-6.54 ± 0.5	-5.28 ± 0.2	-6.70 ± 0.2
	α-Eudesmol *	-6.50 ± 0.6	-5.47 ± 0.1	-6.70 ± 0.3
Oxygenated sesquiterpenes	Elemol	-6.49 ± 0.9	-5.02 ± 0.2	-5.90 ± 0.2
	Germacrene D-4-ol	-5.80 ± 0.6	-5.41 ± 0.1	-6.38 ± 0.2
	<i>epi</i> -α-Cadinol	-5.75 ± 0.6	-5.18 ± 0.1	-6.29 ± 0.2
	<i>trans</i> -Nerolidol	-5.70 ± 0.5	-4.62 ± 0.2	-5.34 ± 0.3
	Patchoulol	-5.67 ± 0.2	-4.97 ± 0.1	-6.45 ± 0.2
	Caryophyllene oxide	-5.90 ± 0.5	-5.25 ± 0.1	-6.50 ± 0.3
	Limonene	-7.22 ± 0.2	-4.60 ± 0.4	-5.16 ± 0.1
Monoterpene hydrocarbons	γ-Terpinene	-7.18 ± 0.4	-4.95 ± 0.4	-5.29 ± 0.1
	<i>p</i> -Cymene	-7.16 ± 0.5	-4.89 ± 0.3	-5.34 ± 0.1
	<i>trans</i> -β-Ocimene	-6.47 ± 0.3	-4.62 ± 0.1	-4.81 ± 0.1
	β-Myrcene	-5.98 ± 0.6	-4.08 ± 0.2	-4.72 ± 0.2
	α-Pinene	-5.02 ± 0.3	-4.24 ± 0.1	-5.13 ± 0.1
	Carvacrol	-7.32 ± 0.3	-5.29 ± 0.4	-5.49 ± 0.1
Phenolic compounds	Thymol	-7.03 ± 0.4	-5.31 ± 0.3	-5.48 ± 0.1
	Eugenol *	-6.54 ± 0.5	-5.16 ± 0.4	-5.46 ± 0.3
Oxygenated monoterpenes	Isopulegol *	-6.70 ± 0.6	-4.85 ± 0.2	-5.19 ± 0.1

	Citronellyl acetate	-6.32 ± 0.4	-4.81 ± 0.2	-5.40 ± 0.2
	Geranyl acetate	-6.30 ± 0.5	-5.23 ± 0.2	-5.71 ± 0.2
	Neral	-6.25 ± 0.5	-4.10 ± 0.2	-4.86 ± 0.2
	Geranial	-6.20 ± 0.4	-4.28 ± 0.2	-4.95 ± 0.2
	Citronellol	-6.07 ± 0.3	-4.51 ± 0.2	-5.01 ± 0.1
	Neryl hexanoate	-5.98 ± 0.4	-5.24 ± 0.2	-5.71 ± 0.3
	Geraniol	-5.91 ± 0.5	-4.65 ± 0.2	-5.18 ± 0.1
	Citronellal	-5.75 ± 0.5	-4.03 ± 0.3	-4.72 ± 0.2
	Linalool	-5.72 ± 0.5	-4.31 ± 0.2	-4.91 ± 0.1
	1,8-Cineole	-4.77 ± 0.2	-4.24 ± 0.2	-5.16 ± 0.2
Other oxygenated compounds	<i>n</i> -Decanal	-5.47 ± 0.3	-5.47 ± 0.3	-4.56 ± 0.1
	6-Methyl-5-hepten-2-one	-5.51 ± 0.2	-4.31 ± 0.2	-4.43 ± 0.2

* Compounds marked with an asterisk were identified in the present study, and the other compounds were also identified in a previous study [25].

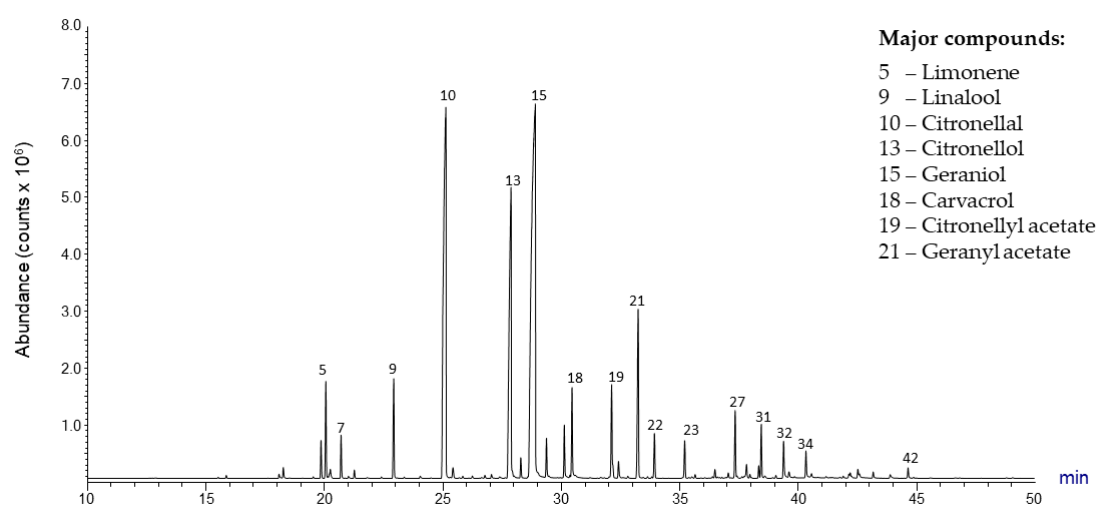


Figure S1. Chromatogram of the blend of seven essential oils used for virucidal activity study. DB-5 capillary column (60 m). Split 1:30. See peak identification in Table 5.