

Bioactive Components of *Myracrodruon urundeuva* against SARS-CoV-2: A Computational Study

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Table S1. Molecular affinity parameters checked by vina method among the chemical constituents of *Myracrodruon urundeuva* and the SARS-CoV-2 proteins (ACE2, M^{Pro}, RBD and Spike)

Parts of the plant	Sl/No.	Compounds	ΔG_{bind}^a (kcal.mol ⁻¹)				Reference
			SPIKE (6VXX)	ACE2 (1R42n)	M ^{Pro} (6lu7)	RBD Spike/ACE2	
	1	Agathisflavone	-9.7	-8.5	-9.3	-9.7	[19]
	2	Alpha Bergamotene	-5.8	-5.0	-5.0	-5.9	[20]
	3	Alpha-pinene	-5.2	-4.7	-4.0	-5.2	[20]
	4	Alpha-terpineol	-6.1	-5.0	-4.8	-5.8	[19]
	5	Aromadendrin	-8.5	-7.0	-7.6	-6.8	[19]
	6	Apigenin	-8.7	-6.7	-7.8	-6.7	[19]
	7	Beta pinene	-5.1	-4.6	-4.6	-5.1	[22]
	8	3-cerene	-5.5	-4.8	-4.2	-5.2	[20]
	9	Caryophyllene oxide	-7.6	-5.7	-5.3	-6.6	[21]
	10	Cianidanol	-7.5	-7.0	-7.2	-6.6	[19]
	11	Eugenol	-5.5	-5.1	-4.8	-5.6	[22]
	12	Gallic acid	-6.3	-5.3	-5.5	-5.9	[19]
	13	Germacrene B	-6.7	-5.6	-5.2	-6.1	[22]
	14	Isoquercitrin	-8.0	-7.6	-8.1	-8.1	[19]
	15	Luteolin	-9.0	-7.1	-7.5	-6.9	[19]

Leaf	16	Limonene	-5.3	-4.9	-4.4	-5.8	[20]
	17	Linalool	-5.2	-4.3	-4.1	-4.6	[20]
	18	Methyl gallate	-6.2	-5.1	-5.6	-5.9	[20]
	19	Myrcenol	-4.4	-4.0	-4.0	-5.1	[20]
	20	Nerolidol	-6.1	-5.1	-4.5	-4.9	[20]
	21	Quercetin	-9.0	-7.4	-7.5	-7.0	[19]
	22	Quercitrin	-8.1	-8.0	-9.0	-7.6	[19]
	23	Spathulenol	-7.2	-6.0	-5.6	-6.4	[21]
	24	Sylvestrene	-5.6	-5.0	-4.7	-5.4	[22]
Bark	25	4-Hydroxy-N-methyl proline	-5.2	-4.4	-5.6	-4.7	[22]
	26	Beta Sitosterol	-7.9	-6.9	-6.3	-7.1	[22]
	27	Cryptochlorogenic acid	-8.6	-7.2	-7.6	-7.3	[22]
	28	4-p-Coumaroylquinic acid	-8.5	-7.0	-4.6	-7.2	[22]
	29	Feruloyl-D-quinic acid	-8.6	-7.0	-7.5	-7.1	[22]
	30	Gallocatechin	-8.6	-7.1	-7.2	-6.6	[22]
	31	Gallocatechin gallate	-8.7	-8.2	-9.0	-7.9	[22]
	32	Galloylquinic acid	-8.4	-6.6	-6.7	-6.9	[22]
Seed	33	Alpha-Elemene	-8.4	-6.0	-5.0	-5.7	[20]
	34	Beta-Chamigrene	-6.6	-5.8	-5.2	-6.1	[20]
	35	Beta-Guaiene	-7.2	-6.3	-5.3	-6.3	[20]
	36	Ethyl	-4.6	-4.3	-4.0	-5.1	[20]
	37	Geranylacetone	-5.5	-4.9	-4.4	-5.6	[20]
	38	Methyl-2-benzoate	-5.8	-4.6	-4.4	-5.5	[20]
	39	Patchoulane	-6.5	-5.7	-5.3	-6.6	[20]
Root	40	Eriodictiol	-8.9	-7.1	-7.3	-6.9	[23]
	41	Mercaptan	-5.6	-4.7	-4.8	-4.3	[23]
	42	Naringenin	-8.7	-7.8	-8.0	-7.5	[23]
	43	Taxifolin	-9.0	-7.1	-7.4	-6.9	[23]
	44	Trihydroxyflavone	-8.3	-6.7	-7.9	-6.7	[23]