

# Phytochemical Profiling, In Vitro Biological Activities, and In Silico Molecular Docking Studies of *Dracaena reflexa*

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**Table S1.** Tyrosinase inhibition (%) of kojic acid (standard) and extract/fractions of *Dracaena reflexa*.

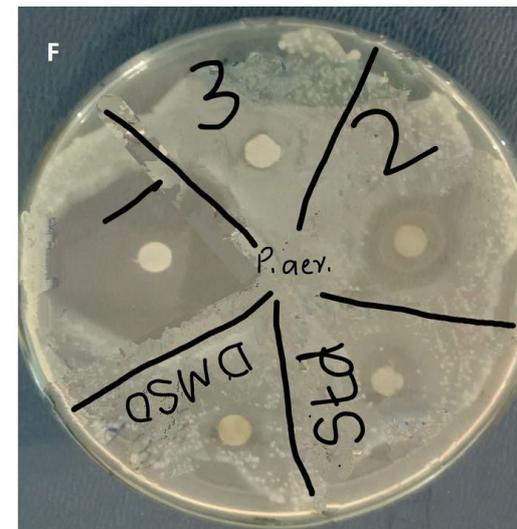
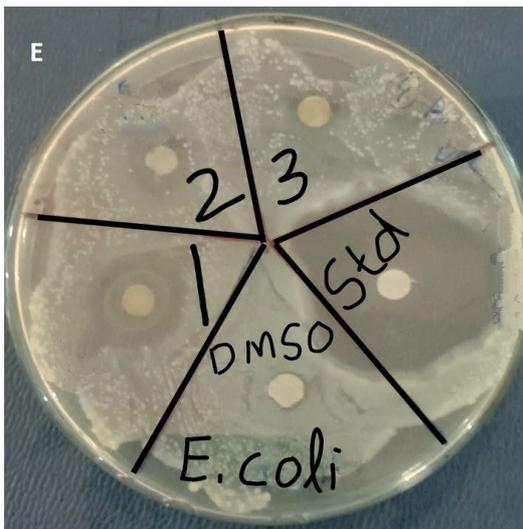
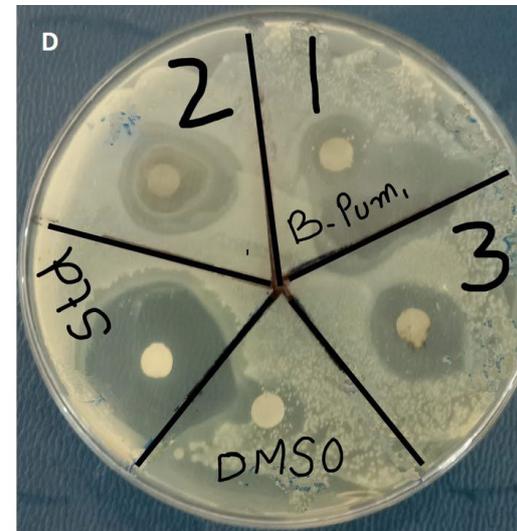
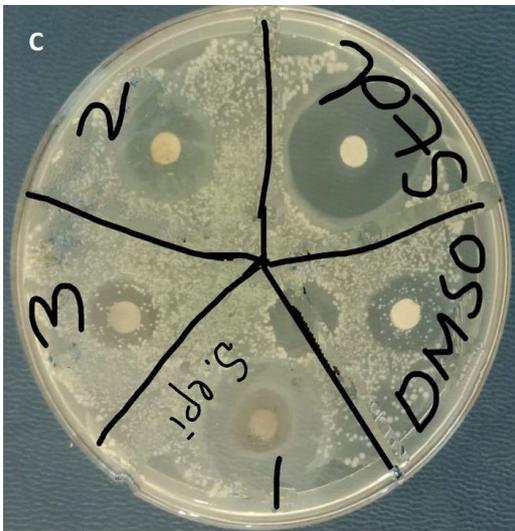
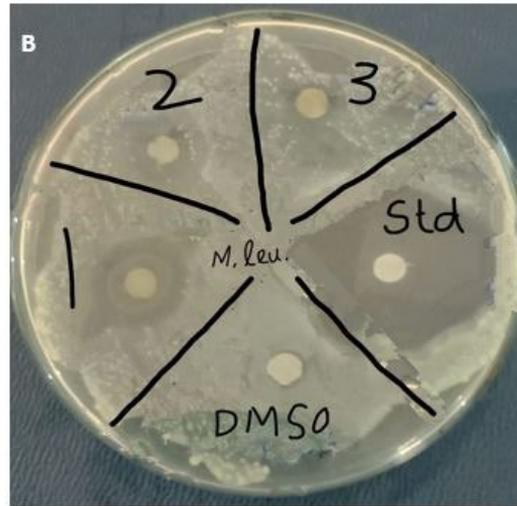
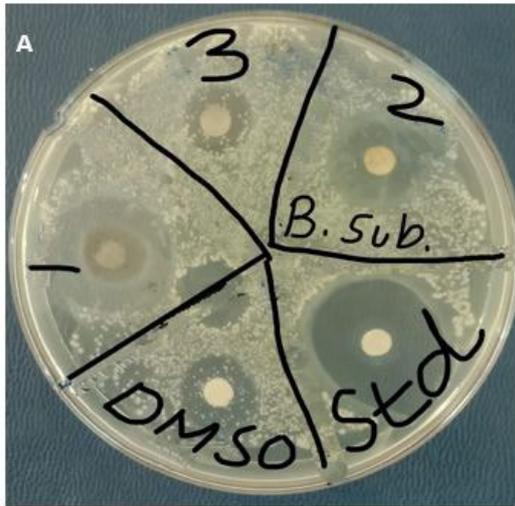
Sample Name	% Inhibition of Tyrosinase
DRME	72.79±1.10
DRHF	61.66±0.9
DRCF	56.03±0.0.75
DRBF	73.46±0.80
Kojic Acid	83.12±1.80

"DRME" Methanolic extract, "DRHF" *n*-hexane fraction, "DRCF" chloroform fraction, and "DRBF" *n*-butanol fraction.

**Table S2.** Acetylcholinesterase and butyrylcholinesterase inhibition (%) of Gantamine (standard) and extract/fractions of *Dracaena reflexa*.

Sample Name	% Inhibition of AChE	% Inhibition of BChE
DRME	56.07±1.25	50.97±0.63
DRHF	48.09±0.94	42.88±1.35
DRCF	40.47±1.85	38.67±2.57
DRBF	64.06±2.65	48.38±1.86
Galantamine	82.58±1.58	53.671±0.97

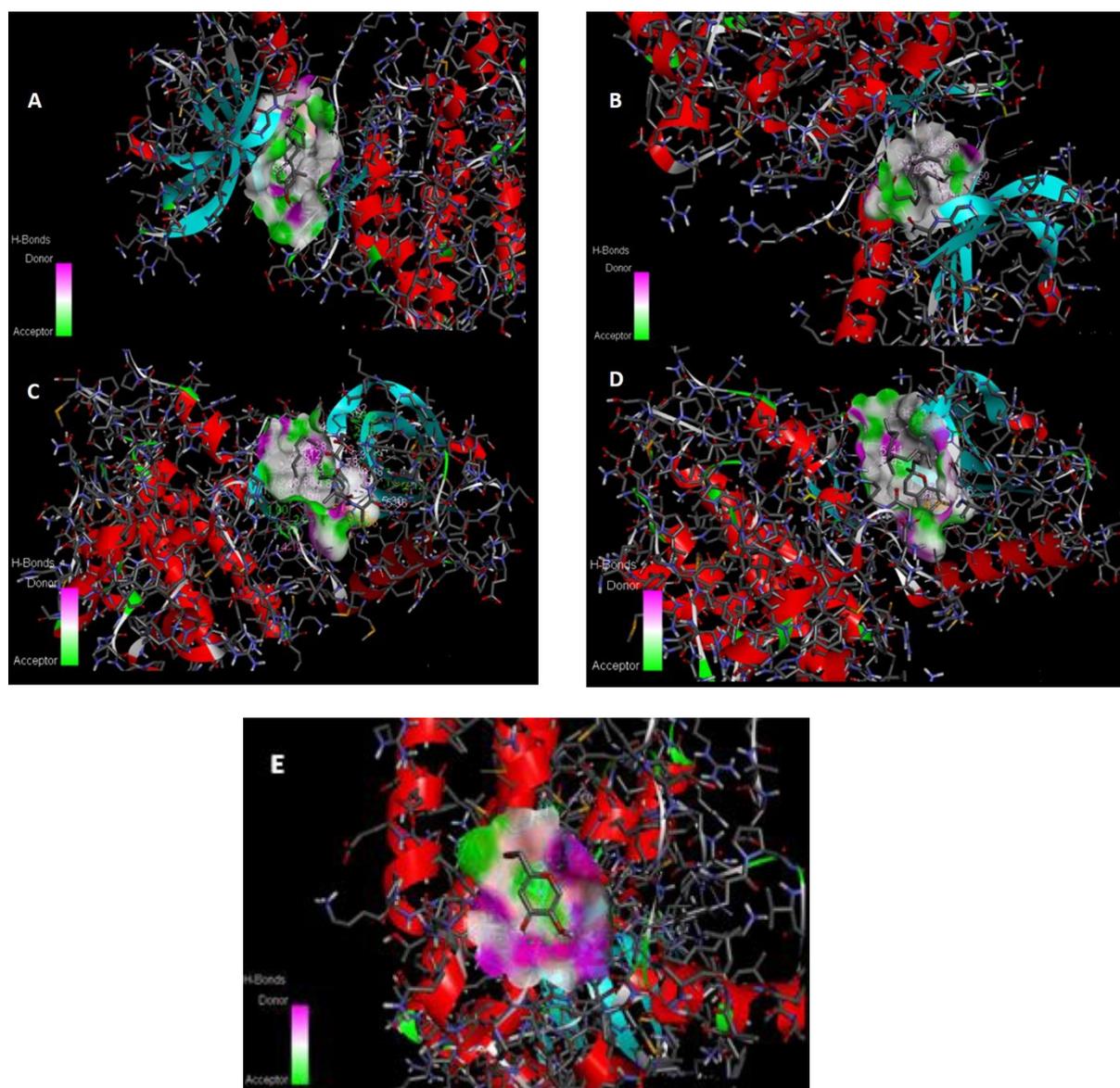
"DRME" Methanolic extract, "DRHF" *n*-hexane fraction, "DRCF" chloroform fraction, and "DRBF" *n*-butanol fraction.



**Figure S1.** Antibacterial activity of *n*-hexane fraction of *D.reflexa* by disc diffusion method against some bacterial strains. "B. sub; *Bacillus Subtilis*, M. leu; *Micrococcus luteus*, S.epi; *Staphylococcus epidermidis*, B.pum; *Bacillus pumilus*, E.coli; *Escherichia coli*, P.aer; *Pseudomonas aeruginosa* 1; 20 mg/mL fraction solution, 2; 10 mg/mL fraction solution, 3; 5 mg/mL fraction solution".

**Table S3.** Binding affinity and intermolecular forces of Kojic acid, Beta-sitosterol, Octadecadienoic acid, Octadecatrienoic acid methyl ester, and Vitamin E with tyrosinase enzyme.

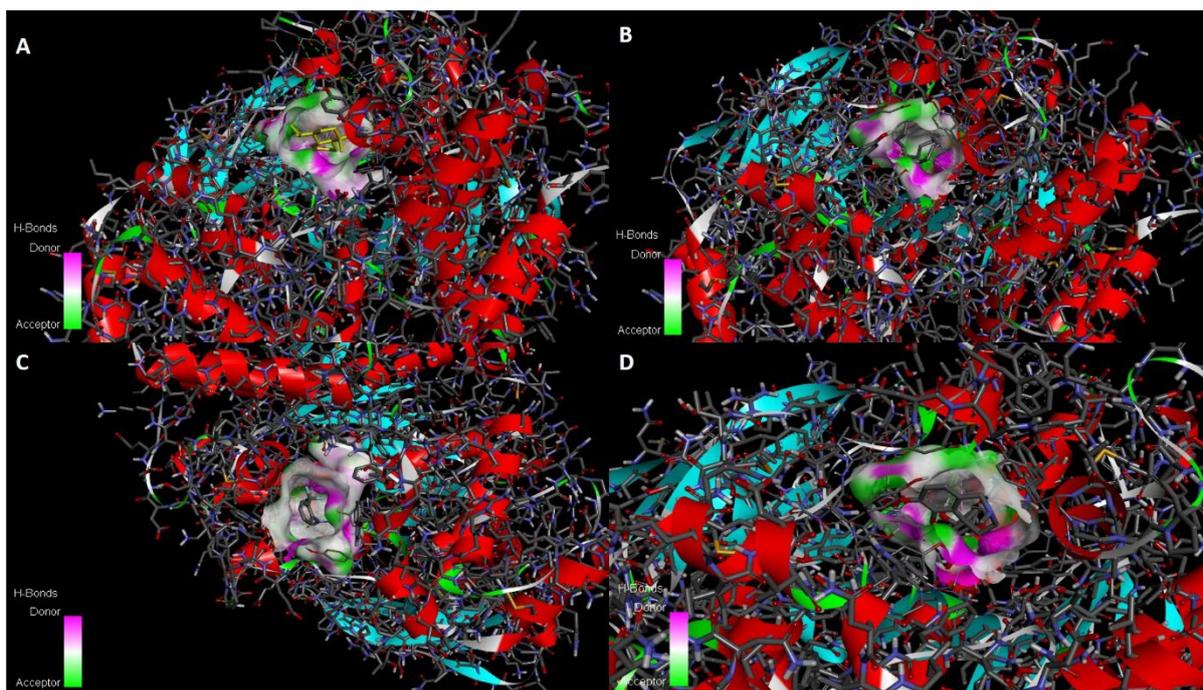
Ligand	Binding Affinity (Kcal/mol)	Amino Acid Interaction			
Beta-Sitosterol	-9.2	<b>Vander Waals</b> GLY:567 ASN:568 ASP:641 ILE:545 ALA:640 MET:535		<b>Alkyl</b> LEU:484 LYS:514 VAL:492 LEU:630	
9,12-Octadecadienoic acid	-5.6	<b>Vander Waals</b> LYS:514 GLU:531 MET:535 GLU:562		<b>Hydrogen bond</b> ASP:641 PHE:642 GLY:643	<b>Alkyl bond</b> LEU:484 VAL:492 ALA:512 ILE:545 VAL:561 ALA:640
Octadecatrienoic acid, methyl ester	-5.8	<b>Vander Waals</b> GLU:531 MET:535 GLU:562 PHE:642	<b>Hydrogen bond</b> ASP:641	<b>Pi alkyl</b> LEU:484 VAL:492 ALA:512 ILE:545 ALA:564 LEU:630 ALA:640	
Vitamin E	-7.8	<b>Vander Waals</b> GLY:485 GLU:486 GLY:487 ALA:512 GLU:531 MET:535 VAL:559 GLU:562 ALA:564 GLY:567 ALA:640	<b>Pi anion</b> ASP:641	<b>Pi sigma</b> VAL:561	<b>Pi alkyl</b> LEU:484 VAL:492 LYS:514 ILE:545
Kojic Acid(standard)	-4.8	<b>Vander Waals</b> GLY:716 ASP:735 TRP:737 HIS:738		<b>Hydrogen bond</b> ARG:718 MET:731 ARG:734 ALA:739	



**Figure S2.** 3D Interaction of tyrosinase and ligands. "A" Beta-Sitosterol, "B" 9,12-Octadecadienoic acid, "C" Octadecatrienoic acid, methyl ester, "D" Vitamin C, and "E" Kojic acid.

**Table S4.** Binding affinity and intermolecular forces of Galantamine, Alpha-cadinol, n-hexadecanoic acid, and N-hydroxy-N'-[2-(trifluoromethyl)phenyl]pyridine-3-carboximidamide (HTPP) with acetylcholinesterase (AChE).

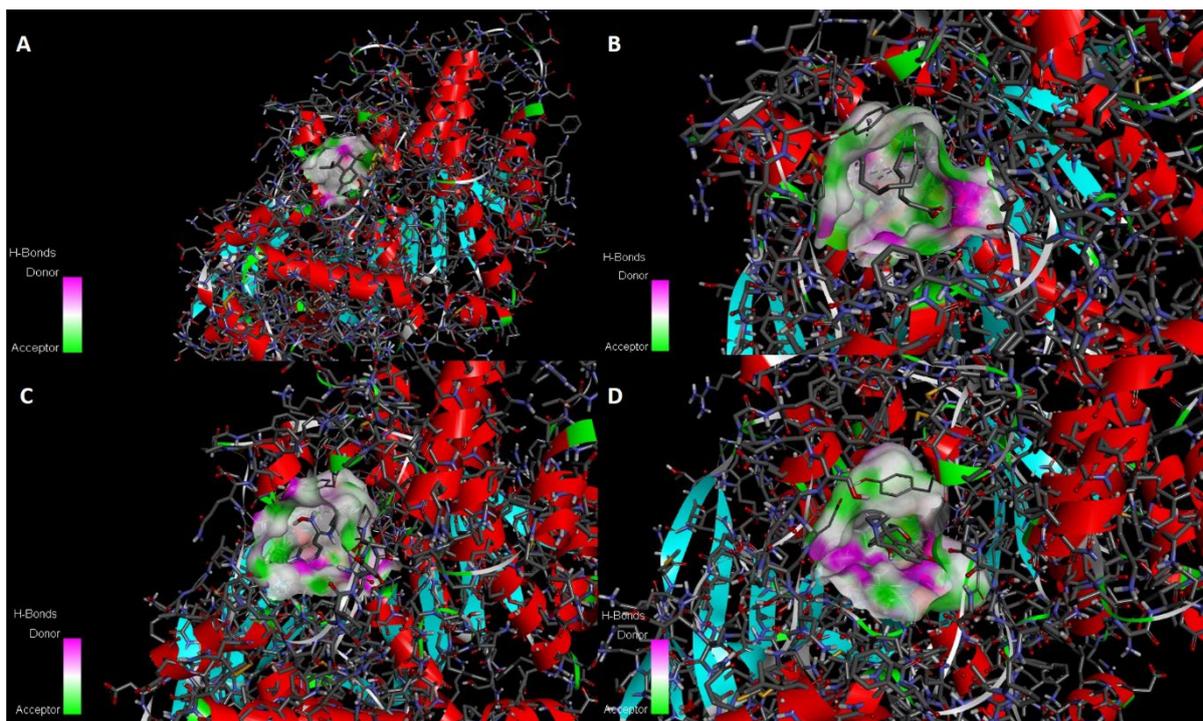
Ligand	Binding Affinity (Kcal/mol)	Amino Acid Interaction			
Alpha-Cadinol	-7.8	<b>Vander Waals</b> Tyr 70 Asp72 Asn 85 Gly 117 Gly 118 Tyr 121 Ser 122 Gly 123 Ser 124 Tyr 130 Phe 330 Phe 331 His 440		<b>Alkyl</b> Trp 84 Leu 127	
<i>n</i> -Hexadecanoic Acid	-6.4	<b>Vander Waals</b> Asp 72 Ser 81 Trp 114 Ser 122 Glu 199 Ser 200 Tyr 334 Trp432 Gly 441 Tyr 442		<b>Hydrogen bond</b> Gly 117 Tyr 130	<b>Pi alkyl</b> Trp 84 Tyr 121 Phe 331 His 440
N-hydroxy-N'-[2-(trifluoromethyl)phenyl]pyridine-3-carboximidamide	-9.3	<b>Vander Waals</b> Asp 72 Gly 117 Gly 118 Gly 119 Gly 123 Ser 124 Leu 127 Tyr 130	<b>Hydrogen bond</b> Trp 84 Tyr 121 His 440	<b>Pi alkyl</b> Phe 330 Phe 331	
Galantamine	-8.2	<b>Vander Waals</b> Gln 69 Asp 72 Pro 86 Gly 118 Tyr 121 Gly 123 Tyr 130 Ser 200 Phe 330 Phe 331	<b>Hydrogen Bond</b> Ser 122	<b>C-Hydrogen Bond</b> Trp 84 Asn 85	<b>Pi alkyl</b> Trp 84 His 440



**Figure S3.** 3D Interaction of Acetylcholinesterase and ligands. "A" Alpha-Cadinol, "B" *n*-Hexadecanoic Acid, "C" N-hydroxy-N'-[2-(trifluoromethyl)phenyl]pyridine-3-carboximidamide, and "D" Galantamine.

**Table S5.** Binding affinity and intermolecular forces of Galantamine, Alpha-cadinol, *n*-hexadecanoic acid, and N-hydroxy-N'-[2-(trifluoromethyl)phenyl]pyridine-3-carboximidamide (HTPP) with butyrylcholinesterase (BChE).

Ligand	Binding Affinity (Kcal/mol)	Amino Acid Interaction			
Alpha-Cadinol	-8.2	<b>Vander Waals</b> Asp 70 Gly 115 Gly 116 Tyr 128 Ala 328 Tyr 332 Trp 430 Met 437 Gly 439 Tyr 440		<b>Hydrogen Bond</b> His 438	<b>Pi sigma</b> Trp 82
<i>n</i> -Hexadecanoic Acid	-5.3	<b>Vander Waals</b> Asp 70 Ser 79 Gly 115 Gly 116 Ala 199 Gly 439		<b>Hydrogen bond</b> Gly 117 Glu 197 Ser 198	<b>Pi alkyl</b> Trp 82 Ala 328 Phe 329 Tyr 332 Trp 430 His 439
N-hydroxy-N'-[2-(trifluoromethyl)phenyl]pyridine-3-carboximidamide	-8	<b>Vander Waals</b> Asp 70 Ser 79 Asn 83 Gly 115 Gly 116 Thr 120 Gly 121 Leu 125 Tyr 128	<b>Hydrogen bond</b> Trp 82	<b>Pi alkyl</b> Ala 328	<b>Pi-pi stacked</b> Phe 329
Galantamine	-8.8	<b>Vander Waals</b> Gly 115 Gly 116 Gly 117 Thr 120 Tyr 128 Glu 197 Ala 199	<b>Hydrogen Bond</b> Ser 198 His 438	<b>Pi-pi T shaped</b> Phe 329	<b>Pi alkyl</b> Trp 82 His 398



**Figure S4.** 3D Interaction of Butyrylcholinesterase and ligands. "A" Alpha-Cadinol, "B" *n*-Hexadecanoic Acid, "C" N-hydroxy-N'-[2-(trifluoromethyl)phenyl]pyridine-3-carboximidamide, and "D" Galantamine.