

In silico preliminary evaluation of bioactive compounds from five Unani drugs as potential SARS-CoV-2 inhibitors

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







Supplementary Data

Supplementary Table S1: 2D representation of the interaction between phytochemicals and SARS-CoV-2 Spike (S) glycoprotein (6LZG) and Main Protease3CLpro (7BQY). The ligand is shown in sticks and the interacting amino acid residues with their numbers are shown inside circles. Each colour of amino acid residues and interaction markers indicates different types of interaction.

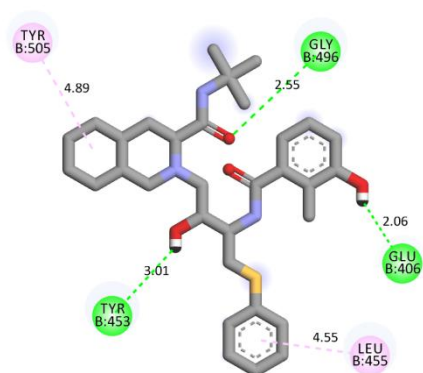
SARS-CoV-2 Spike (S) glycoprotein
Binding Energy (kcal/mol)

SARS-CoV-2 Main Protease (3CLpro)
Binding Energy (kcal/mol)

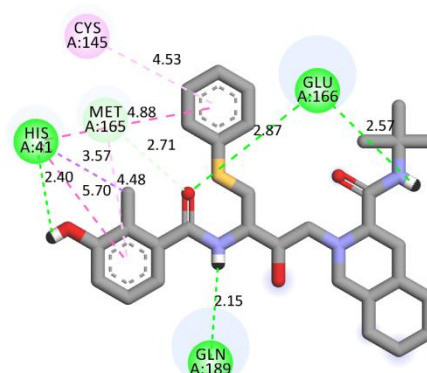
Interactions

	van der Waals		Pi-Sigma
	Conventional Hydrogen Bond		Pi-Sulfur
	Carbon Hydrogen Bond		Pi-Pi T-shaped
	Pi-Donor Hydrogen Bond		Pi-Alkyl

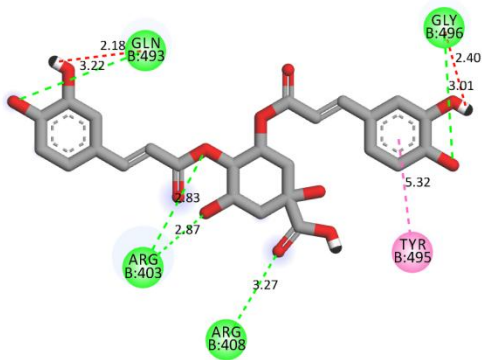
Nelfinavir ΔG -7.2



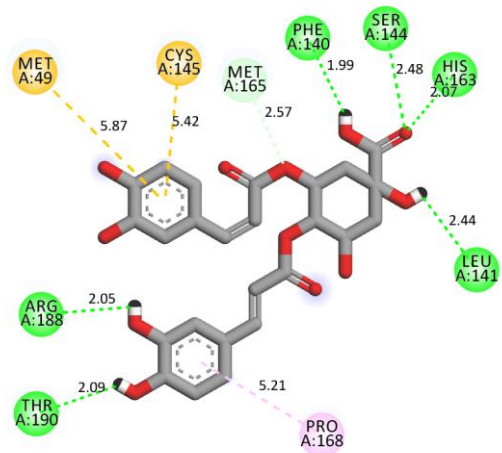
Nelfinavir ΔG -7.7



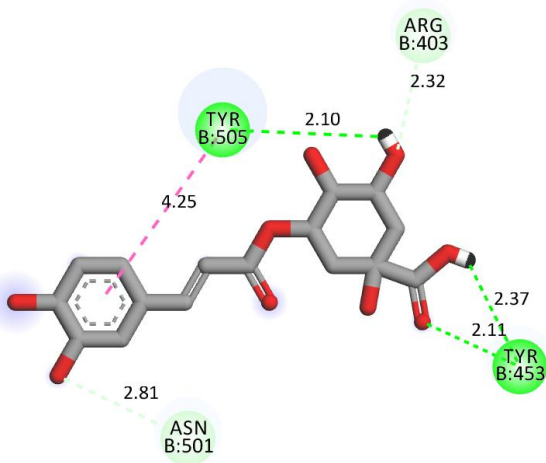
3,4-Dicafeoylquinic acid ΔG -6.6



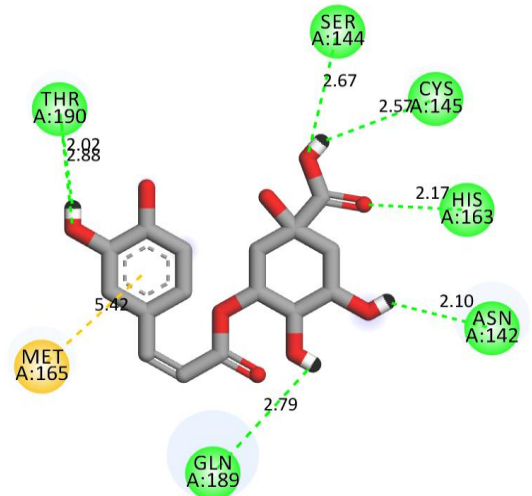
3,4-Dicafeoylquinic acid ΔG -8.7



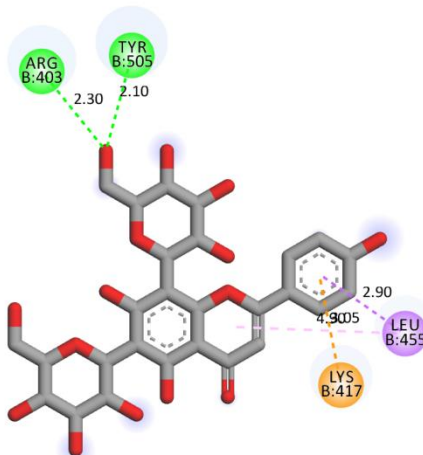
5-O-Caffeoylquinic acid ΔG -7.0



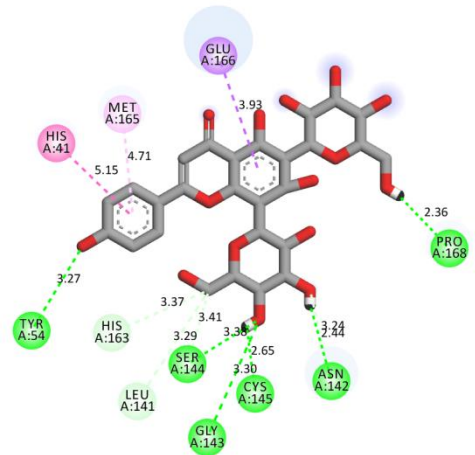
5-O-Caffeoylquinic acid ΔG -7.3

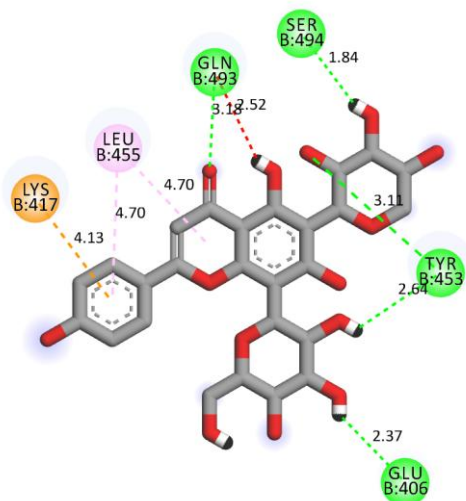
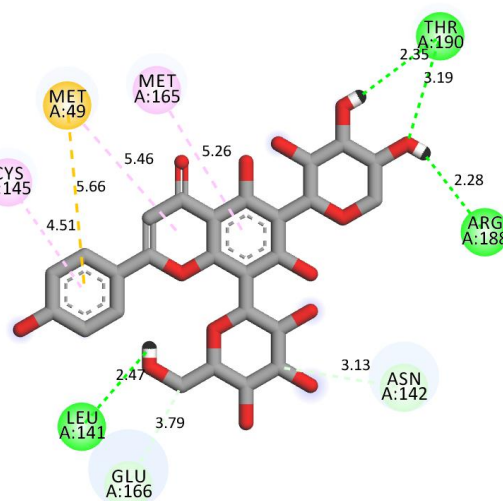
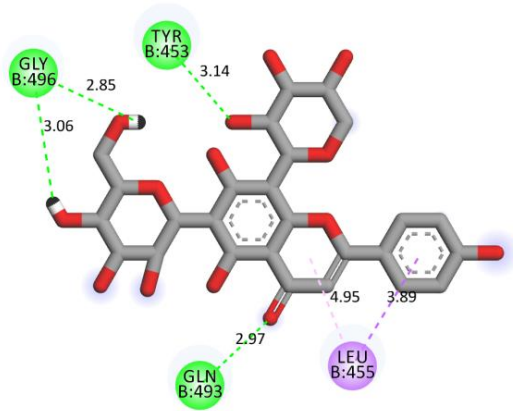
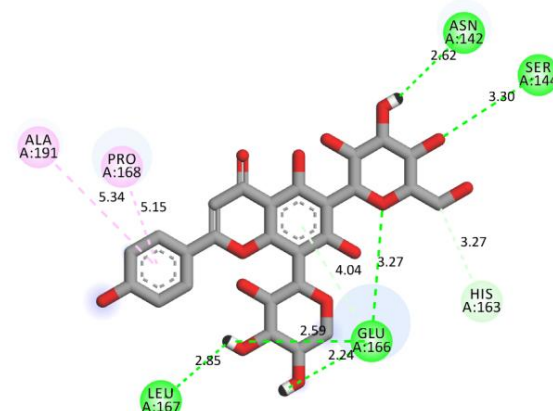
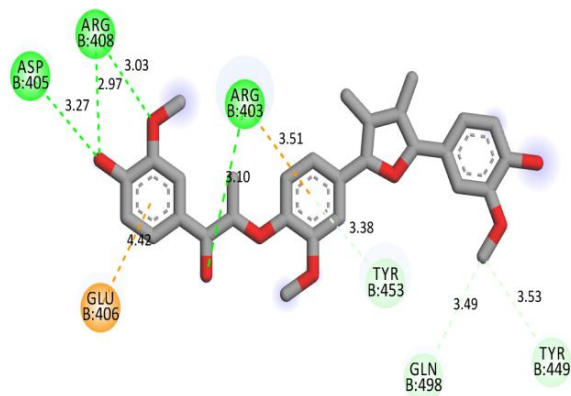
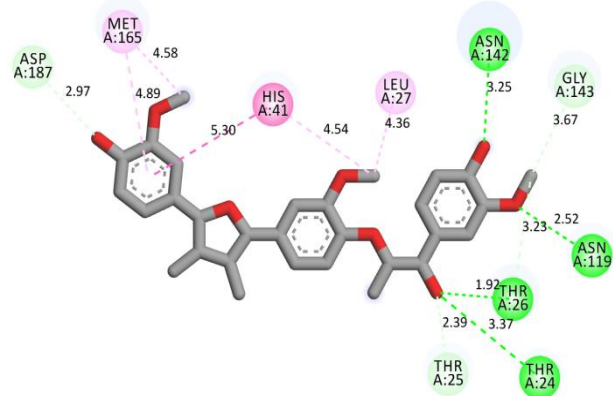


Vicenin-2 ΔG -6.7

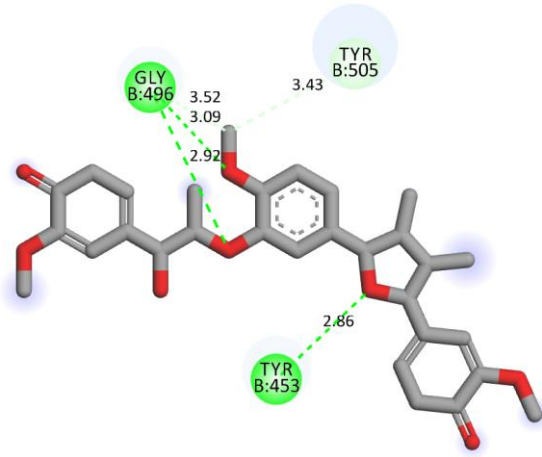


Vicenin-2 ΔG -8.2

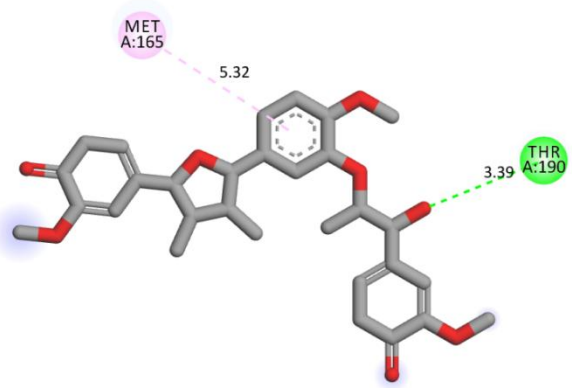


Isoschaftoside ΔG -6.7Isoschaftoside ΔG -8.9Schaftoside ΔG -6.9Schaftoside ΔG -8.3Zijusesquilignan A ΔG -7.2Zijusesquilignan A ΔG -7.8

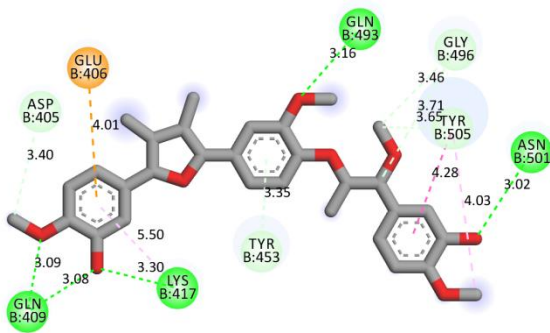
ZijusesquilignanBΔG -7.2



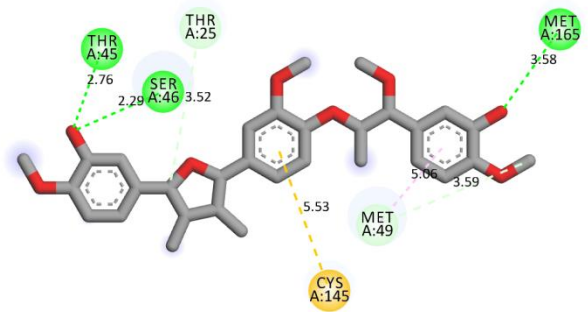
ZijusesquilignanBΔG -6.5



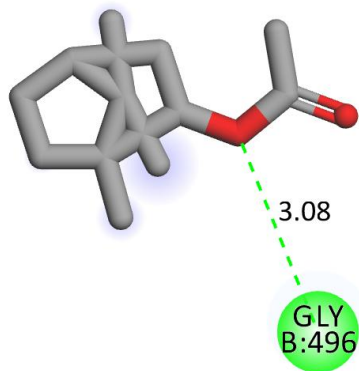
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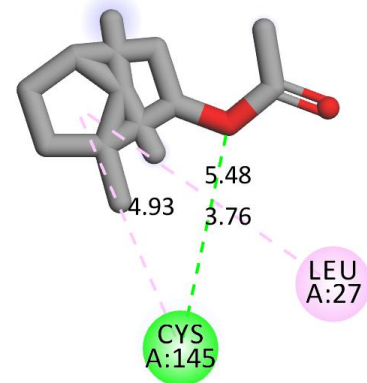
ZijusesquilignanCΔG -7.8

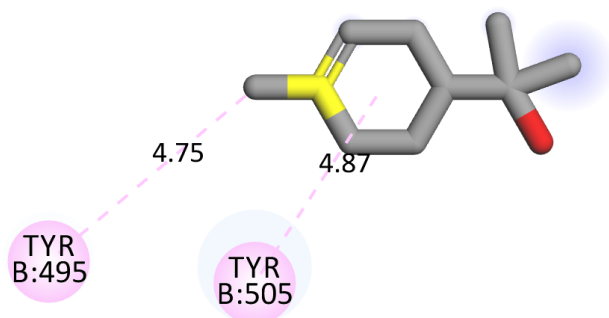
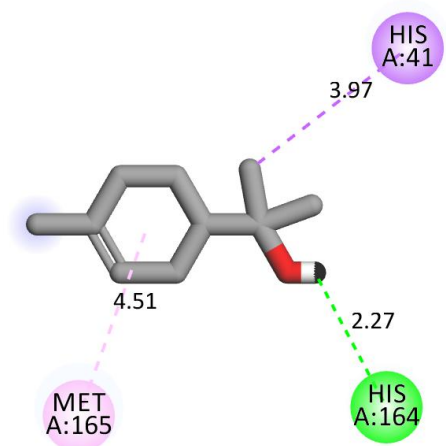
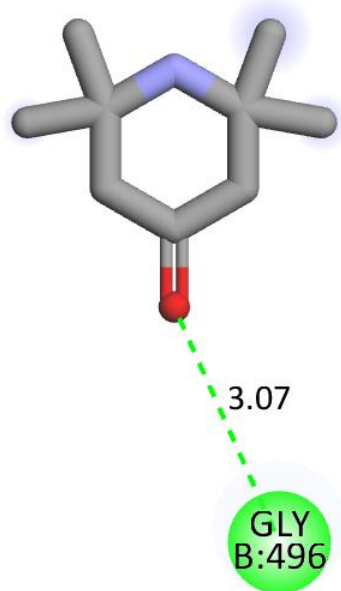
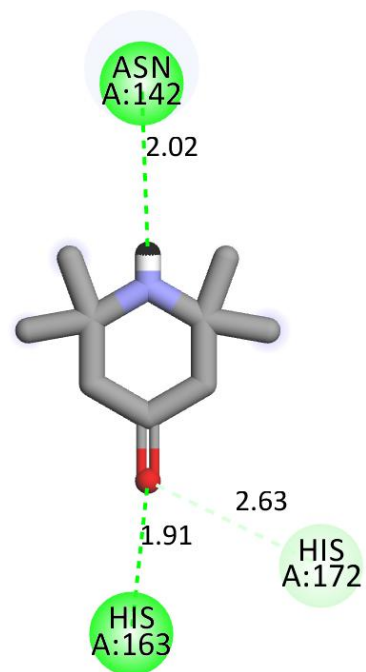


Bornyl acetate ΔG -4.6

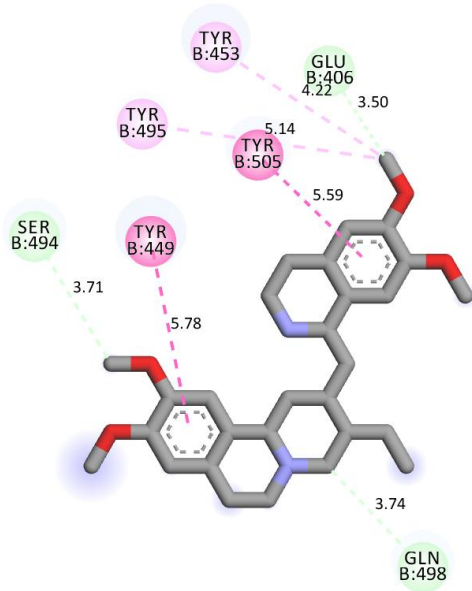


Bornyl acetate ΔG -4.9

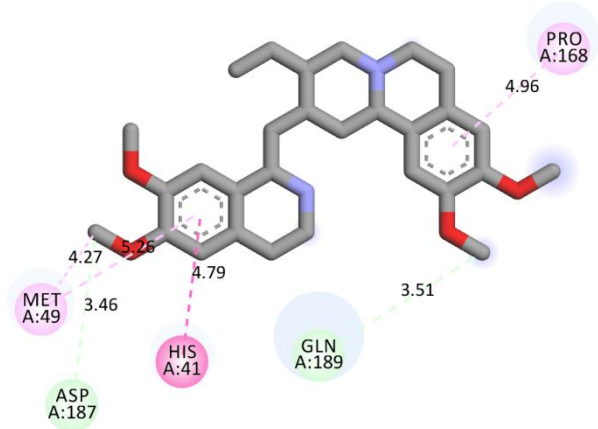


α -terpineol ΔG -5.0 α -terpineol ΔG -4.8Triacetoneamine ΔG -4.8Triacetoneamine ΔG -4.6

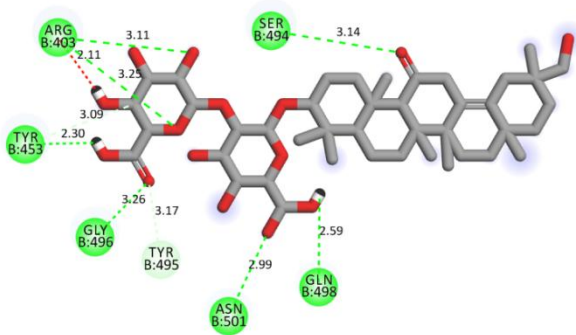
Emetine Δ G -7.3



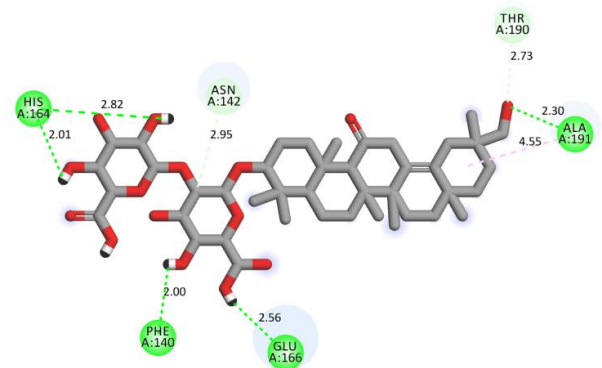
Emetine Δ G -7.8



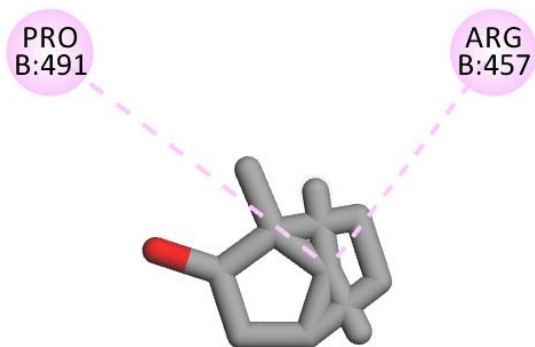
Glycyrrhizin Δ G -7.6



Glycyrrhizin Δ G -7.8



Borneol Δ G -4.7



Borneol Δ G -4.1

