

Supplementary Material

Ethyl Acetate Fraction of *Bixa orellana* and Its Component Ellagic Acid Exert Antibacterial and Anti-inflammatory properties against *Mycobacterium abscessus* subsp. *massiliense*

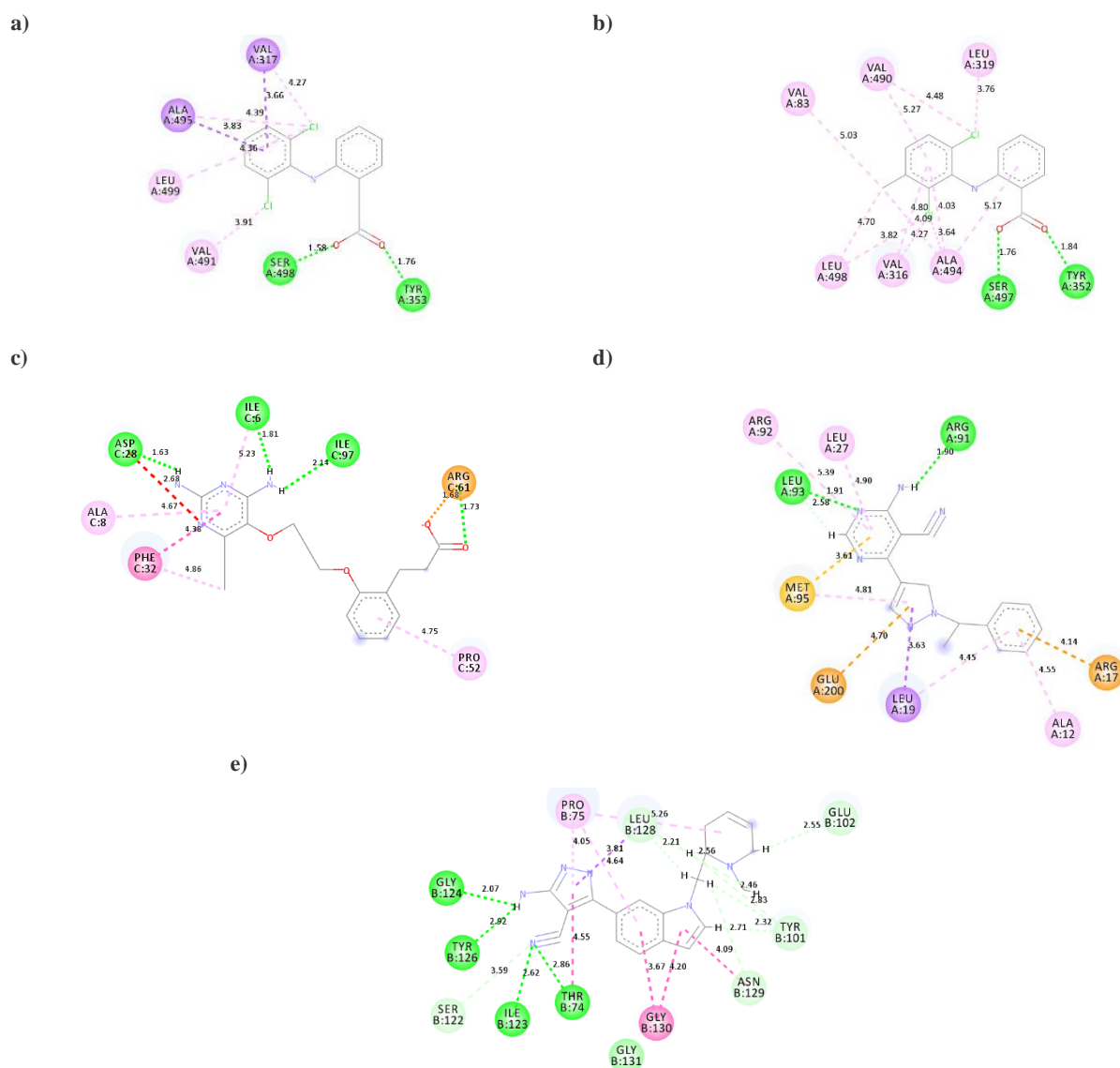


Figure S1: Diagram 2D of Interactions between controls / native ligands and targets: a) diclofenac and COX2 (PDB ID: 1PXX); b) meclofenamic acid and COX2 (PDB ID: 5IKQ); c) MMV ligand and dihydrofolate reductase (PDB ID: 7K6C); d) Q0Q ligand and phosphoribosylaminoimidazole-succinocarboxamide synthase (PDB ID: 6YYB), and e) JD8 ligand and tRNA (guanine-N(1))-methyltransferase (PDB ID: 6QR4). Interactions: Conventional Hydrogen Bond: ■, Pi-Sigma: ■, Alkyl/ Pi-Alkyl: ■, Van der Waals: ■, Salt Bridge: ■ (present in c), Pi-Pi stacked: ■ (present in c), Unfavorable Acceptor-Acceptor: ■, Pi-cation: ■ (present in d), Carbon Hydrogen Bond: ■.

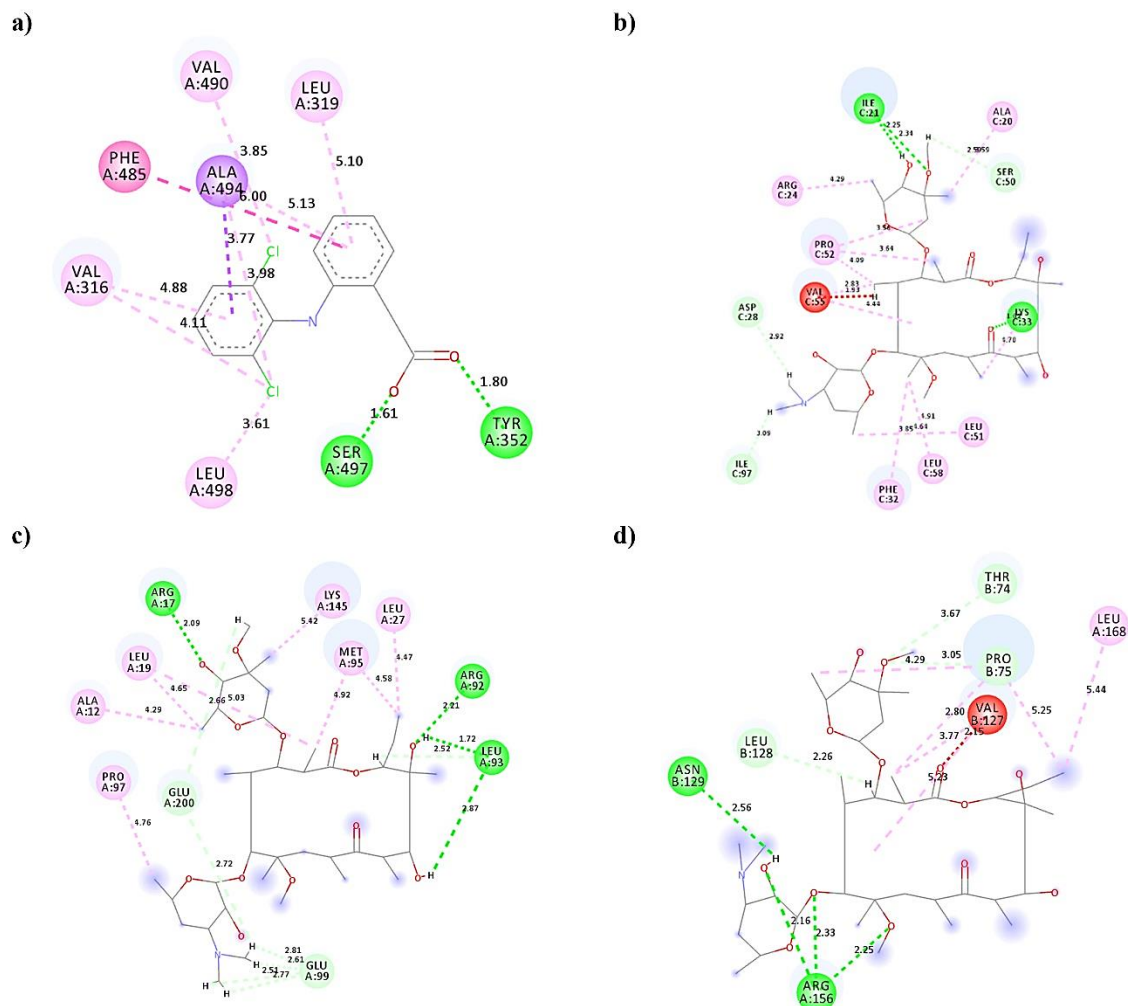


Figure S2: Diagram 2D of Interactions between controls and targets. a) Interactions between diclofenac and COX2 (PDB ID: 5IKQ); b) Interactions between claritromycin and Dihydrofolate reductase (PDB ID 7K6C); c) Interactions between claritromycin and Phosphoribosylaminoimidazole-succinocarboxamide synthase (PDB ID 6YYB); d) Interactions between clarithromycin and tRNA (guanine-N(1)-)-methyltransferase (PDB ID 6QR4).

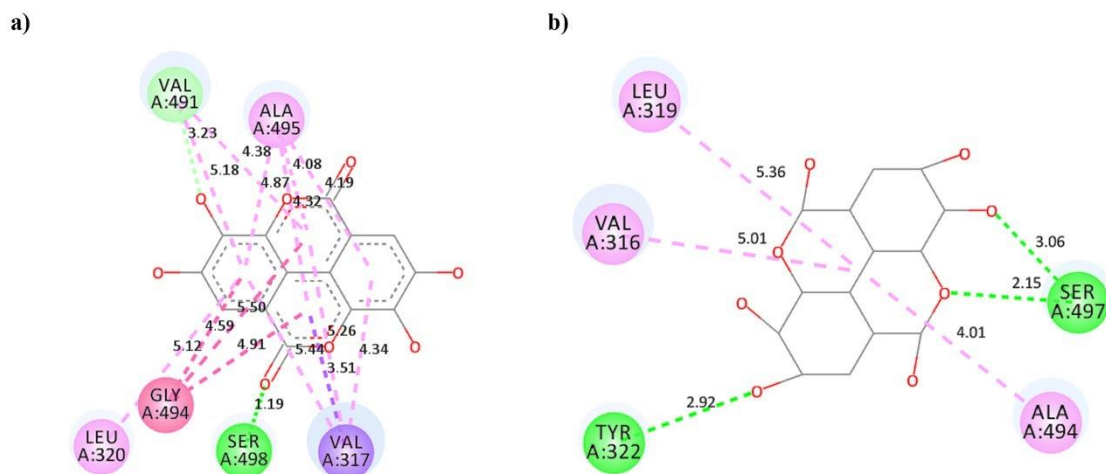


Figure S3: Diagram 2D of Interactions between ellagic acid and COX2 targets: (a) with the murine COX2 (PDB ID: 1PXX) and (b) with the human COX2 (PDB ID: 5IKQ). Interactions: ■ - Conventional Hydrogen Bond, ■ - Pi-Sigma, ■ - Alkyl/ Pi-Alkyl, ■ - Carbon Hydrogen Bond, ■ - Amide Pi-Stacked

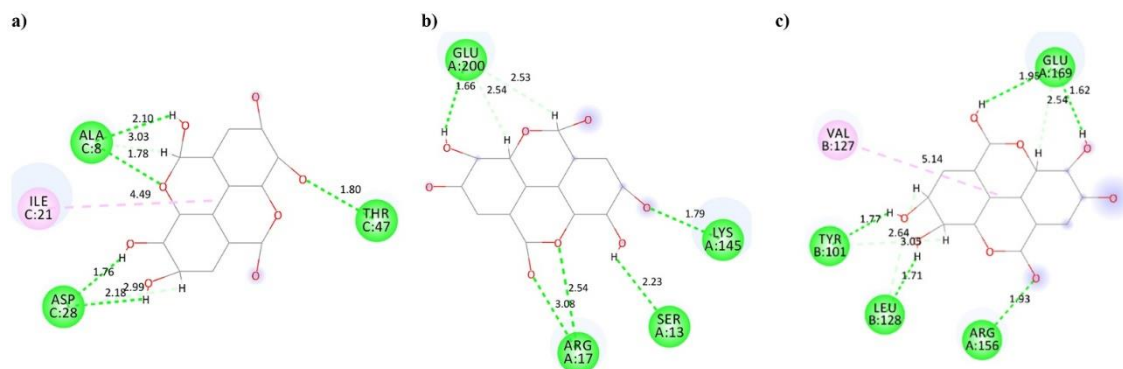


Figure S4: Diagram 2D of Interactions between ellagic acid and targets for antimicrobial activity: a) Dihydrofolate reductase (PDB ID 7K6C); b) Phosphoribosylaminoimidazole-succinocarboxamide synthase (PDB ID 6YYB), and c) tRNA (guanine-N(1)-)-methyltransferase (PDB ID 6QR4). Interactions: ■ - Conventional Hydrogen Bond, ■ - Alkyl, ■ - Carbon Hydrogen Bond.

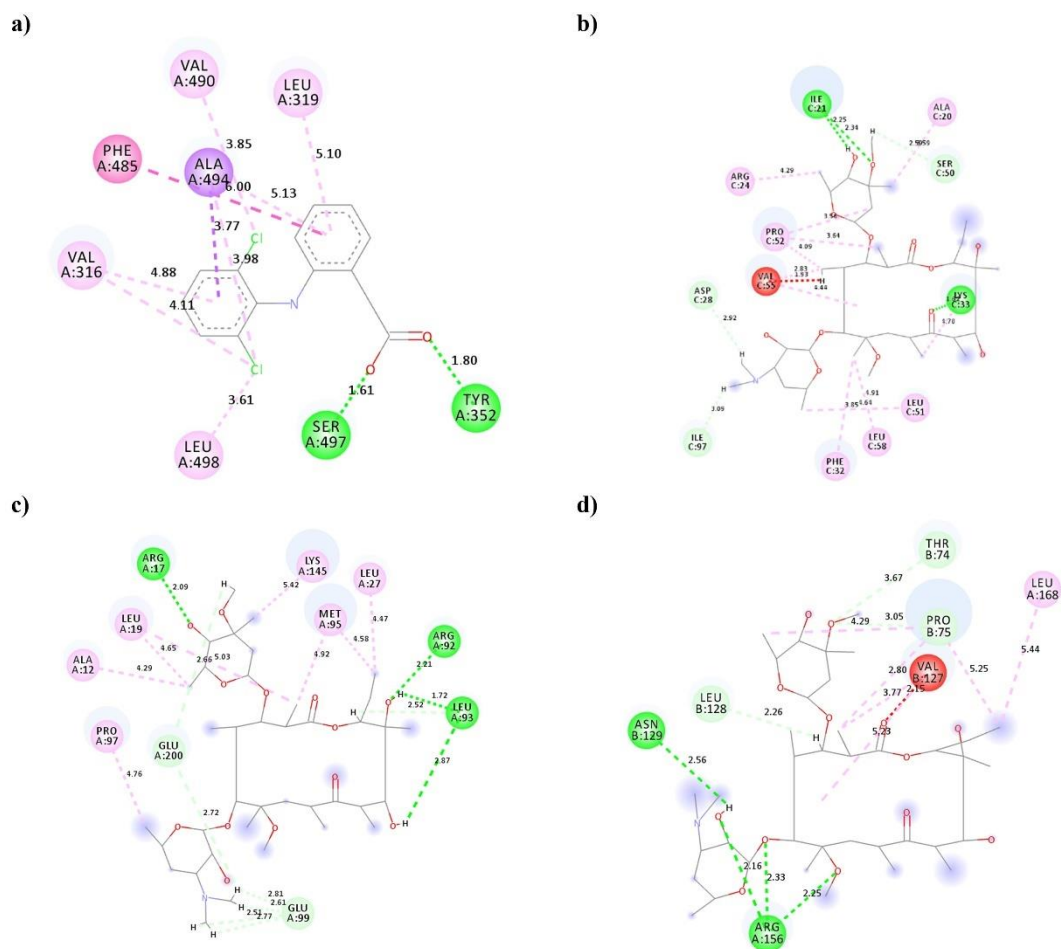


Figure S5: Diagram 2D of Interactions between: a) diclofenac and COX2 (PDB ID: 5IKQ); b) clarithromycin and Dihydrofolate reductase (PDB ID 7K6C); c) clarithromycin and Phosphoribosylaminoimidazole-succinocarboxamide synthase (PDB ID 6YYB), and d) clarithromycin and tRNA (guanine-N(1))-methyltransferase (PDB ID 6QR4).

Table S1: Predicting molecular properties related to Lipinski's rule

Compound	Oral				
	Bioavailability ($< 140 \text{ \AA}^2$)	MW (< 500)	ALogP (≤ 5)	HBD (≤ 5)	HBA (≤ 10)
Clarithromycin	183.726	747.477	2.200	4	14
Diclofenac	50.926	269.149	4.373	2	3
Ellagic Acid	135.723	302.193	1.584	4	8

AlogP = the logarithm of the partition coefficient between n-octanol and water; MW: Molecular Weight; HBD: Hydrogen Bond Donnor; HBA: Hydrogen Bond Acceptor.