

Assessment of the Antioxidant and Antimicrobial Potential of *Ptychotis verticillata* Duby Essential Oil from Eastern Morocco: An In Vitro and In Silico Analysis

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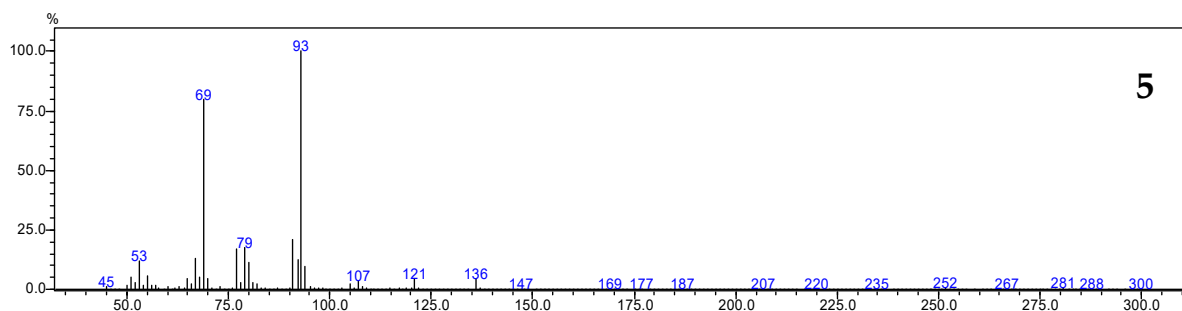
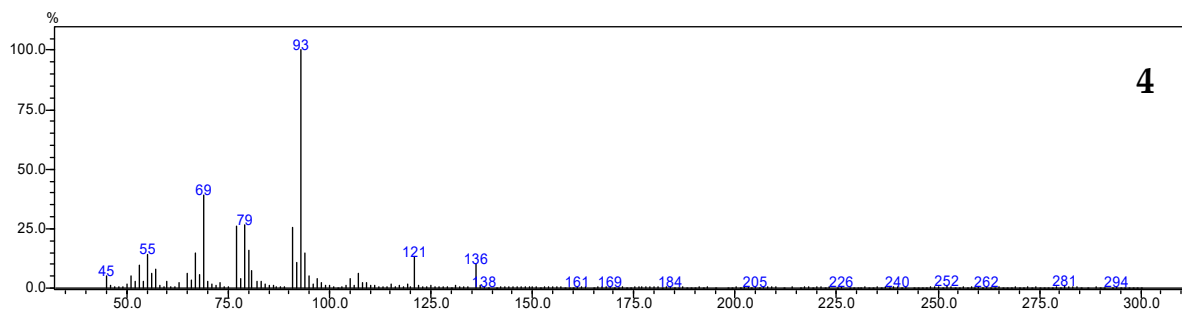
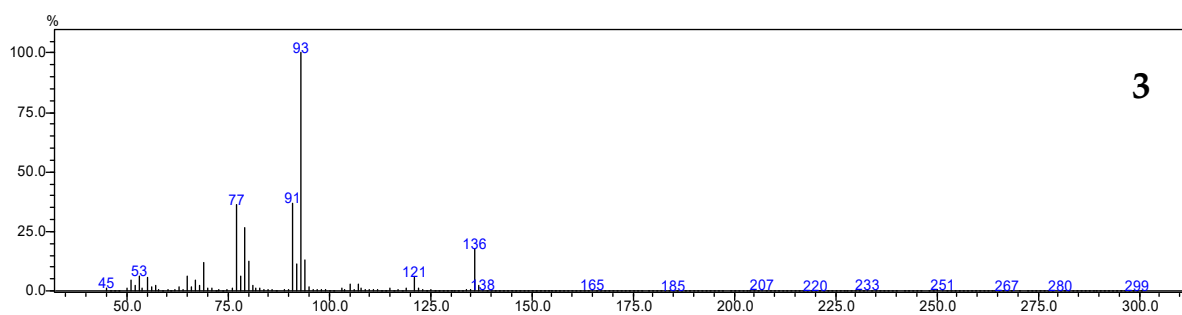
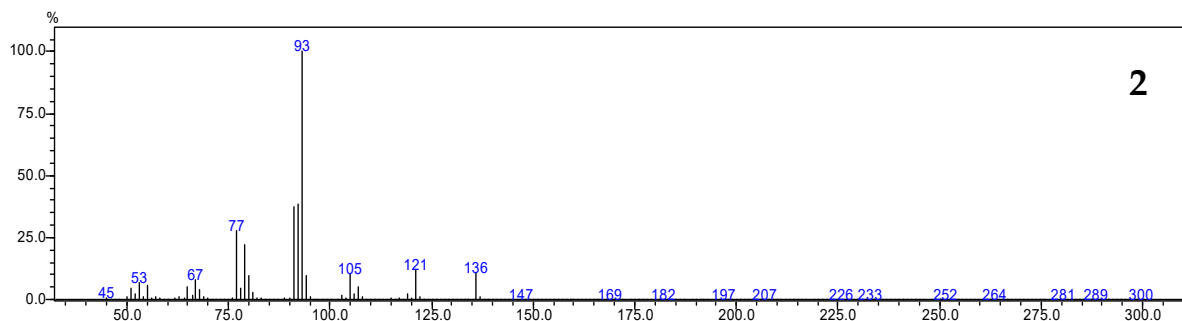
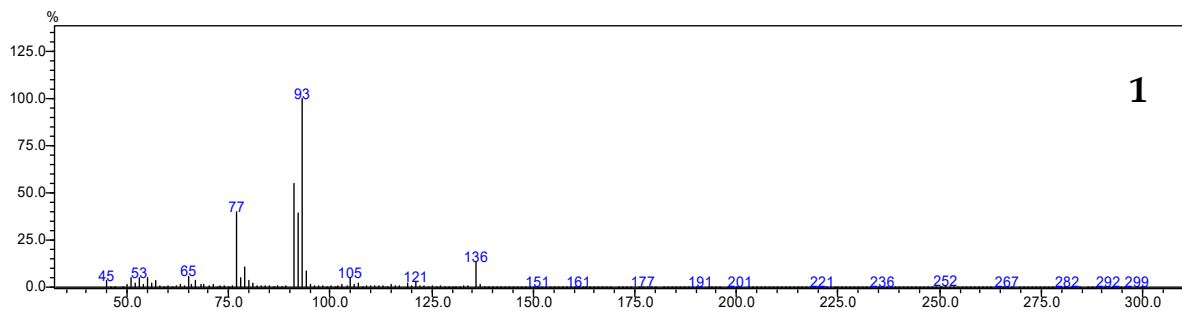
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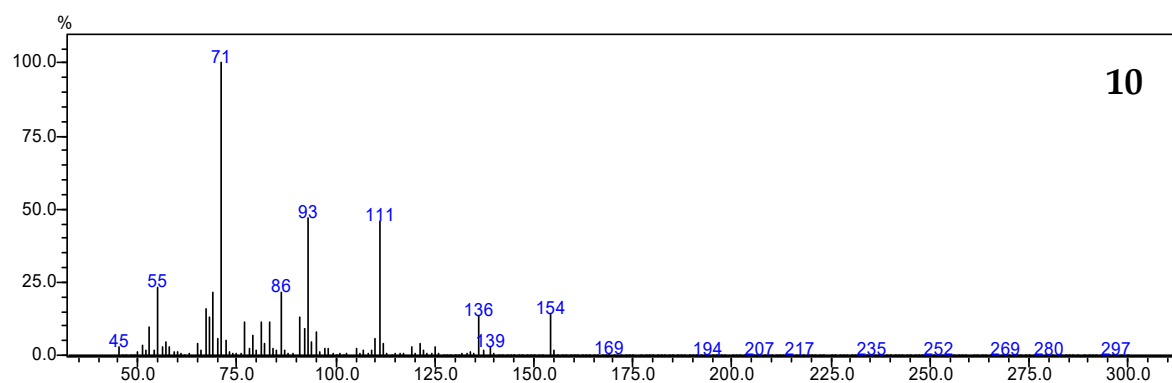
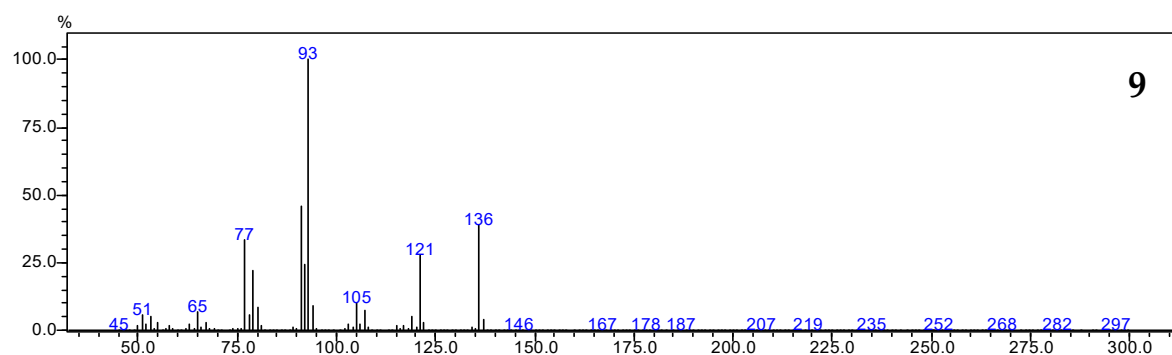
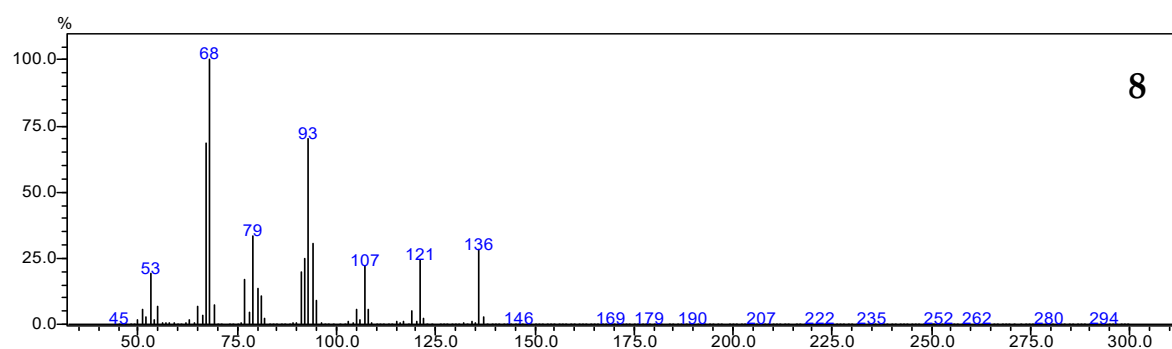
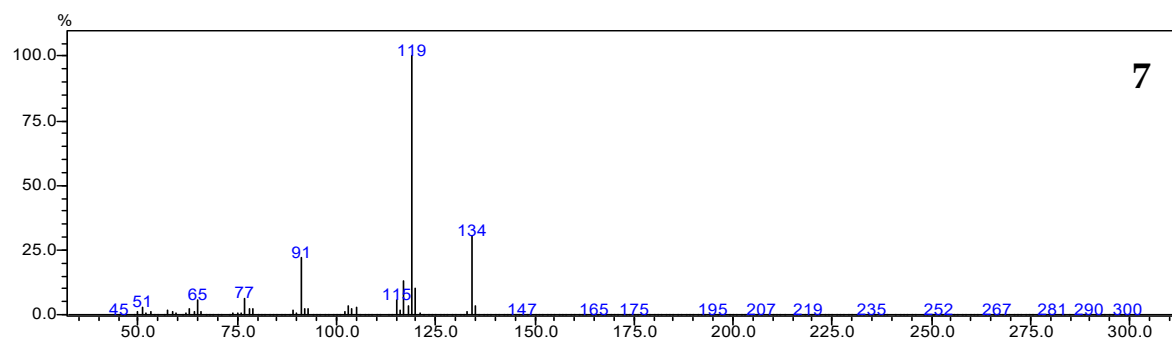
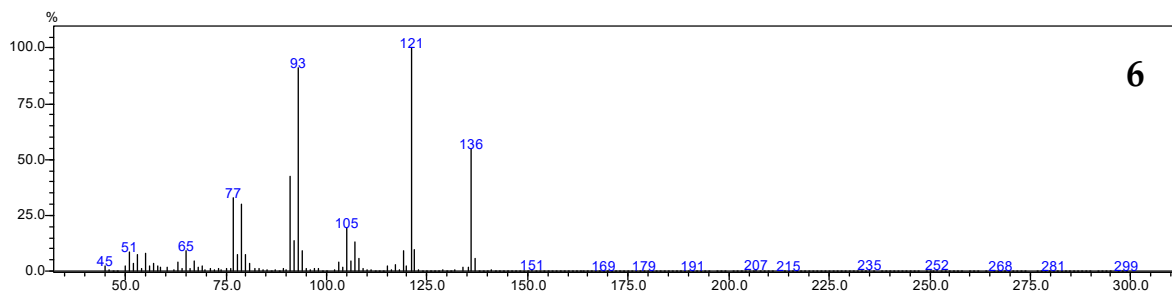
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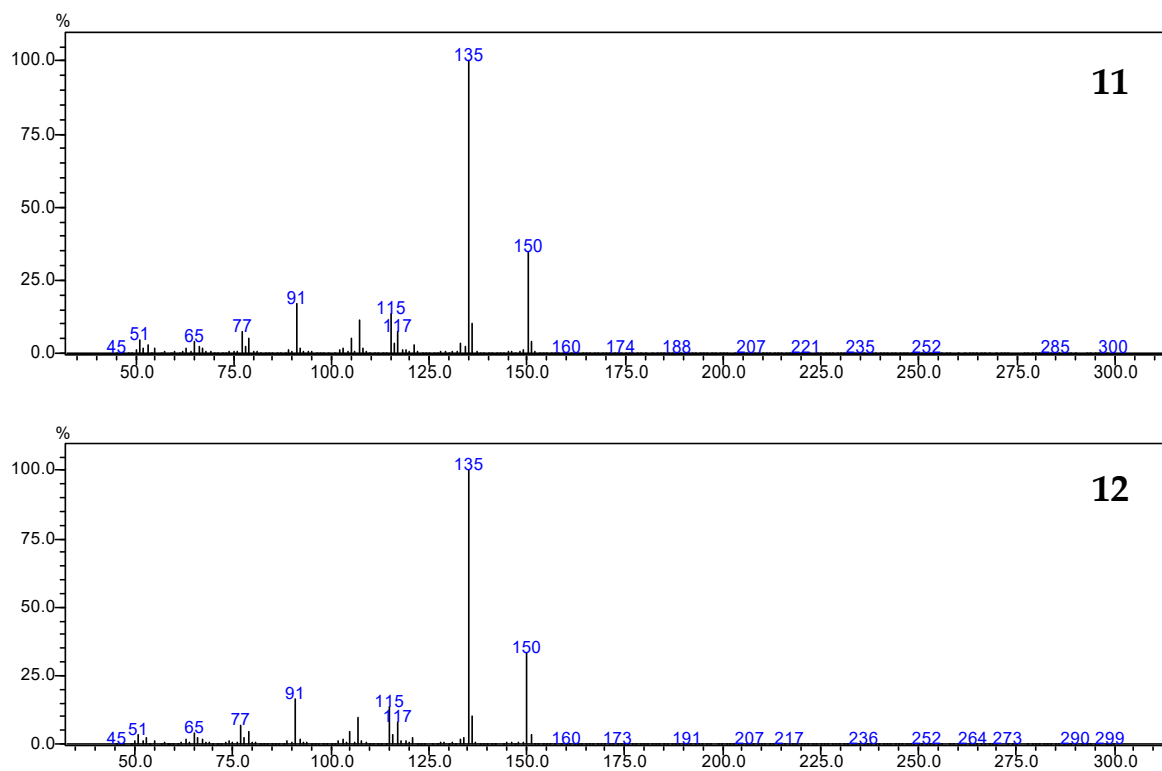


Figure S1. Copies of MS spectra of substances identified in PVEO using GC/MS. **(1)** α -Thujene, **(2)** α -Pinene, **(3)** Sabinene, **(4)** β -Pinene, **(5)** β -Myrcene, **(6)** (+)-4-Carene, **(7)** *m*-Cymene, **(8)** D-Limonene, **(9)** γ -Terpinene, **(10)** *p*-Menth-1-en-4-ol, **(11)** Thymol, **(12)** Carvacrol.

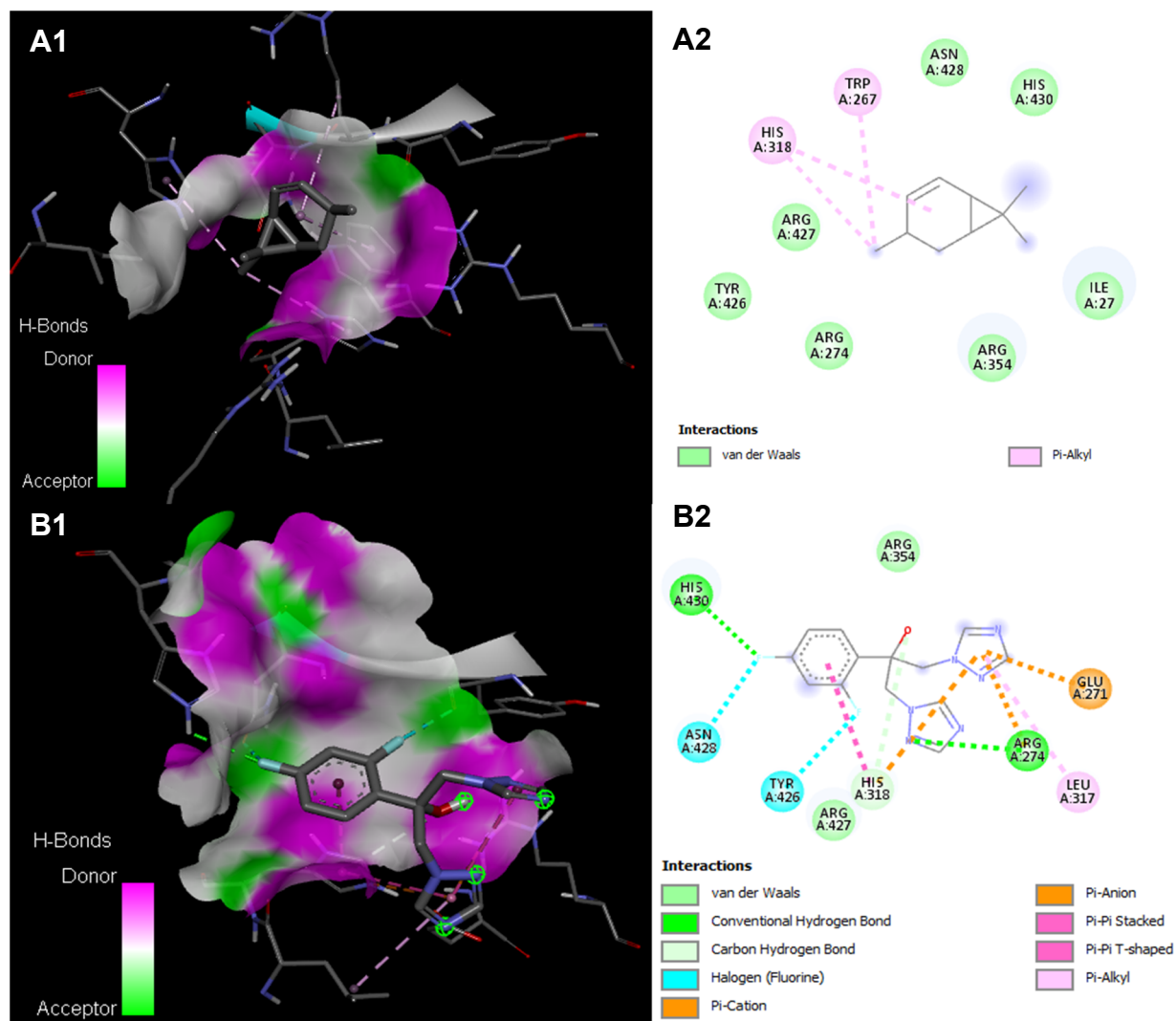
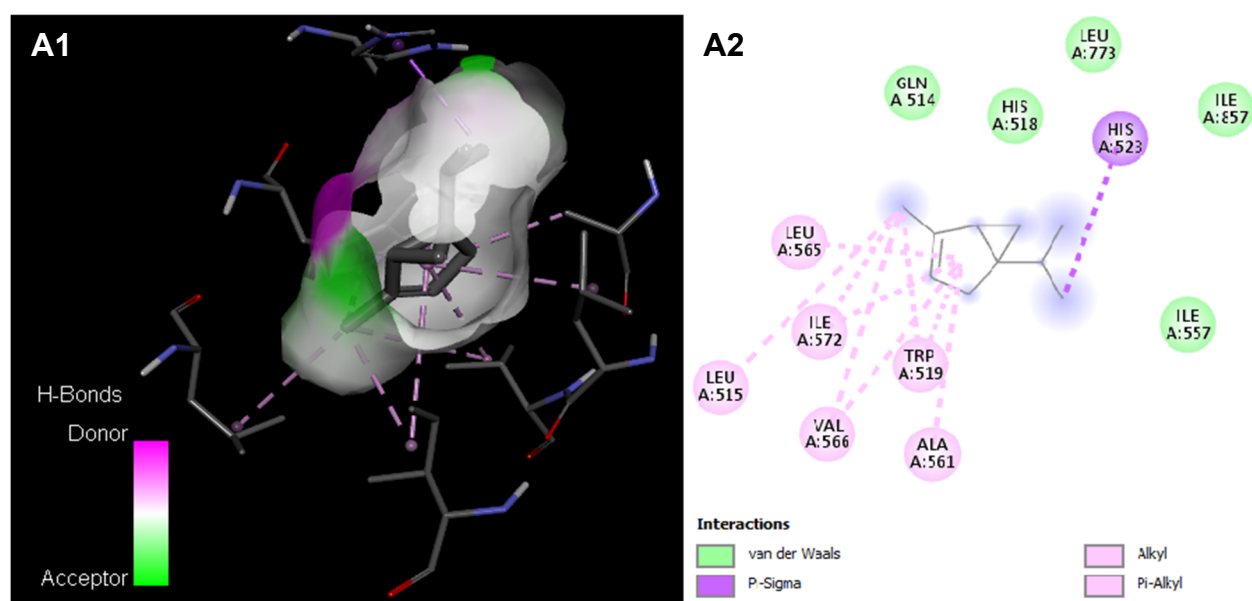


Figure S2. 2D, and 3D schemes of the interactions of 4-(+)-Carene (A1, and A2), the native ligand (Fluconazole) (B1, and B2), with the active site of Cytochrome P450 14 α -sterol Demethylase (PDB ID: 1EA1).



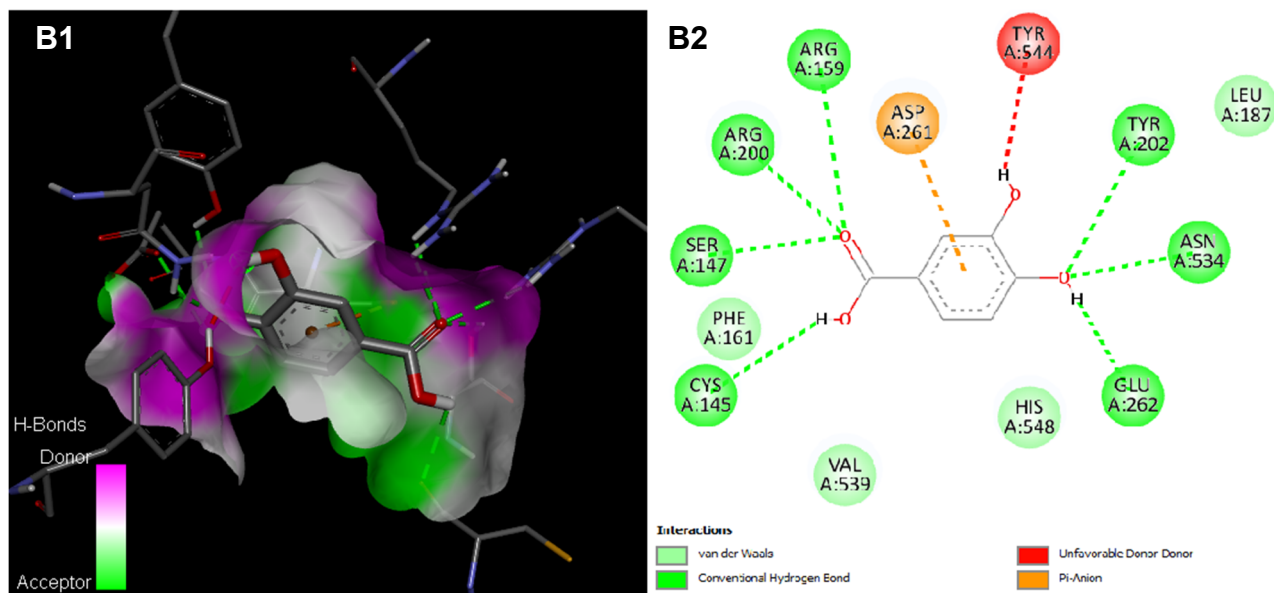
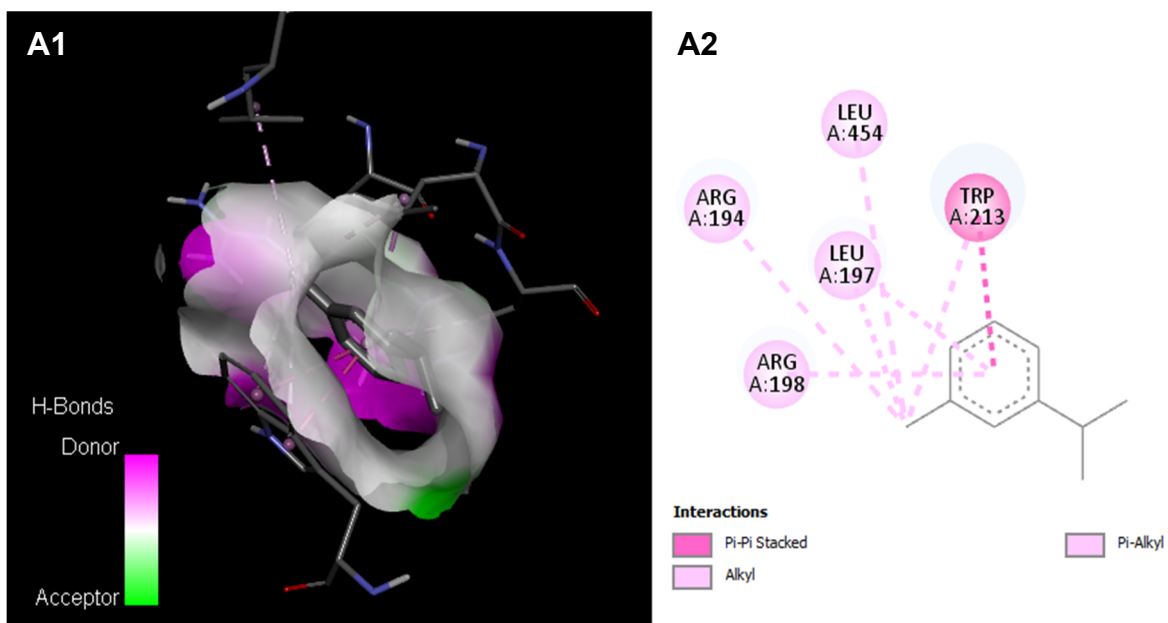


Figure S3. 2D, and 3D schemes of the interactions of α -Thujene (A1, and A2), the native ligand (Protocatechuic Acid) (B1, and B2), with the active site of lipoxxygenase (PDB ID: 1N8Q)



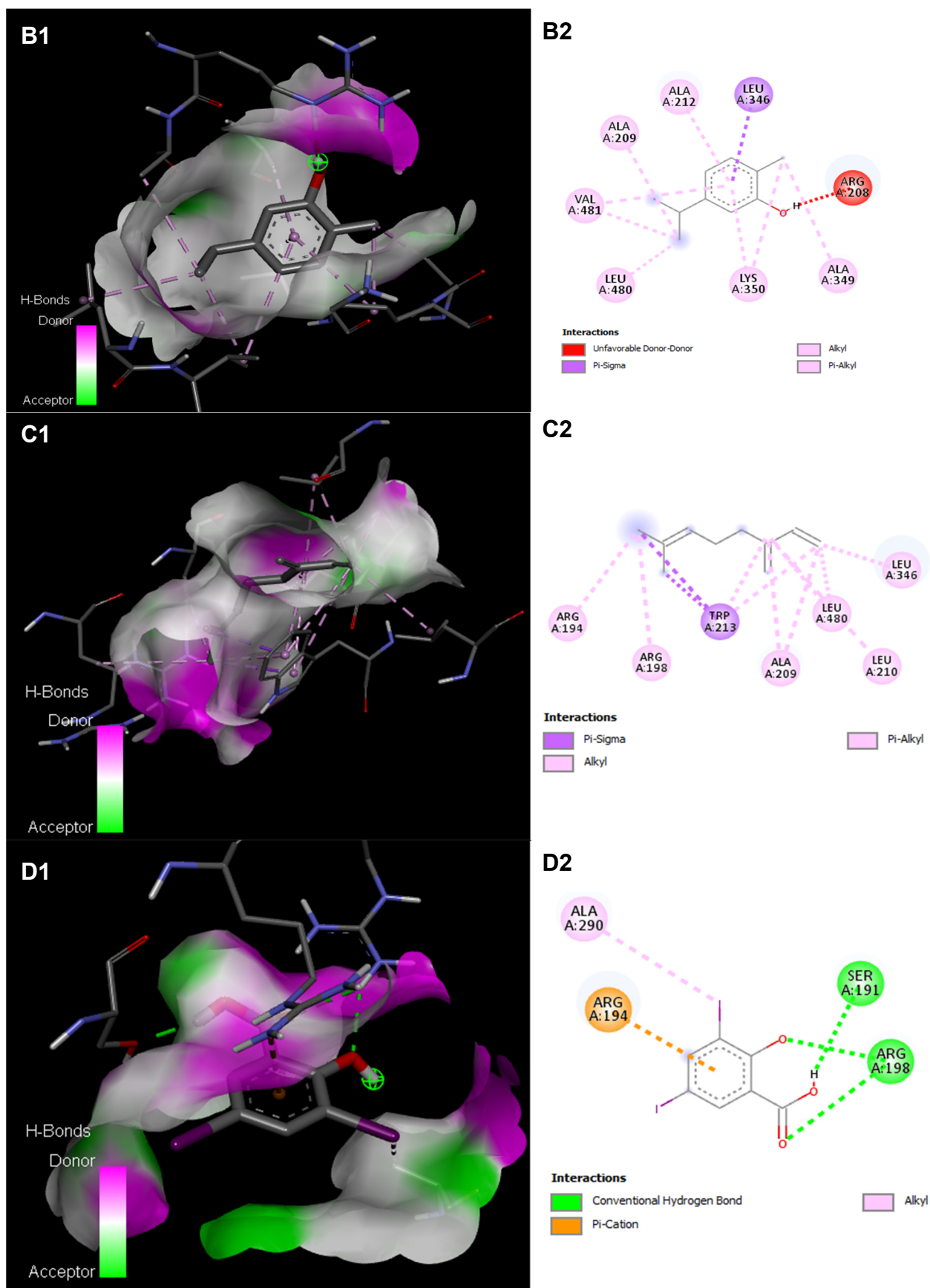


Figure S4. 2D, and 3D schemes of the interactions of *m*-Cymene (A1, and A2), Carvacrol (B1, and B2), β -Myrcene (C1, and C2), and the native ligand (3,5-Diiodosalicylic Acid) (D1, and D2), with the active site of bovine serum albumin (PDB ID: 4JK4)