

Figure S1. The docking poses of Eupalinolide with COX-2 and with interacted amino acids between ligand and COX-2 residues.

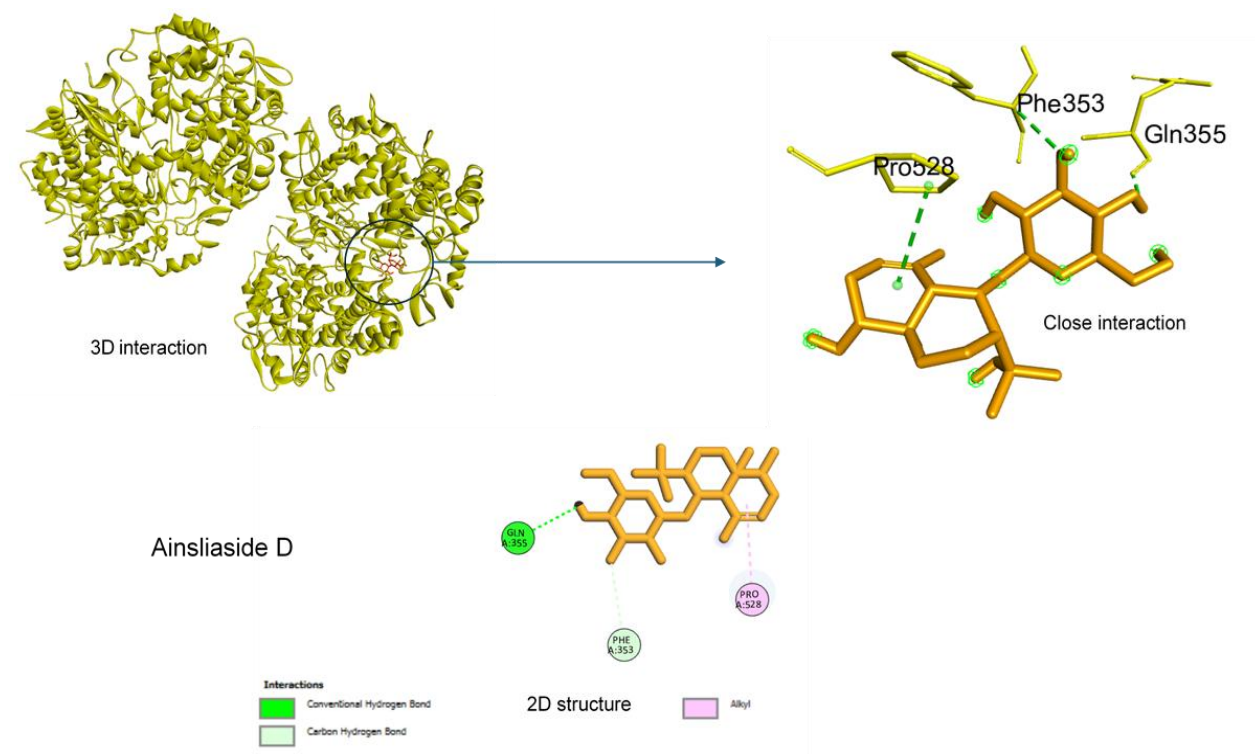


Figure S2. The docking poses of Ainsliaside D with COX-2 and with interacted amino acids between ligand and COX-2 residues.

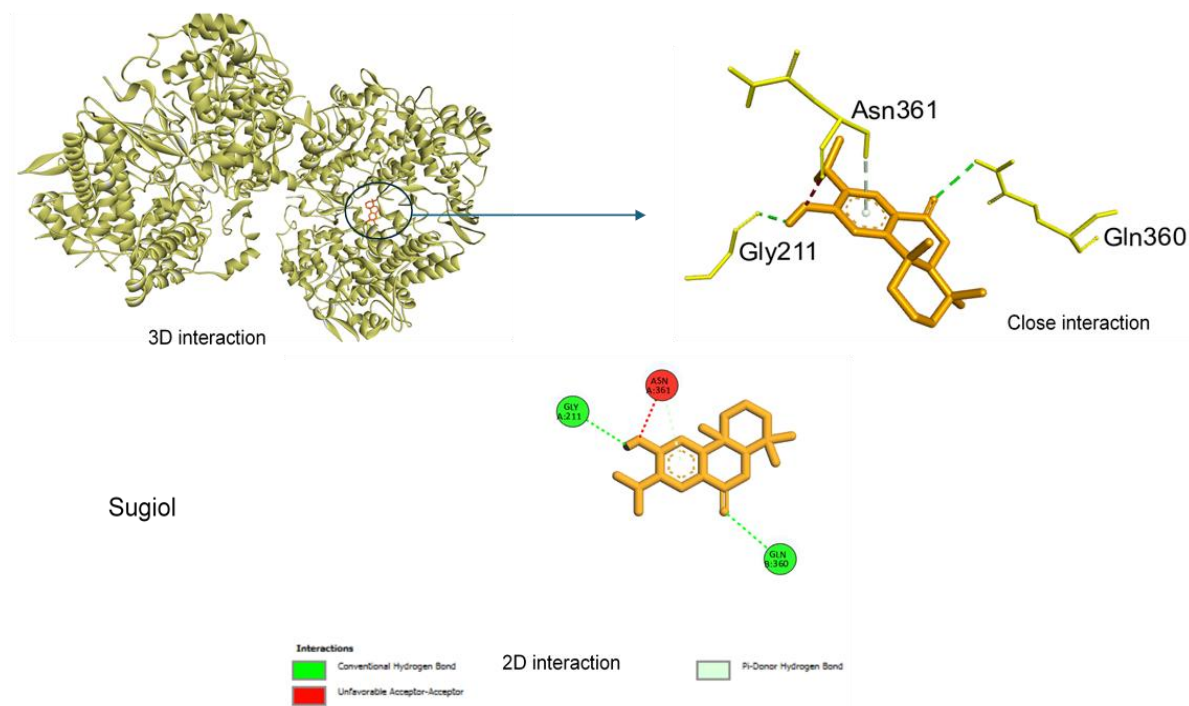


Figure S3. The docking poses of Sugiol with COX-2 and with interacted amino acids between ligand and COX-2 residues.

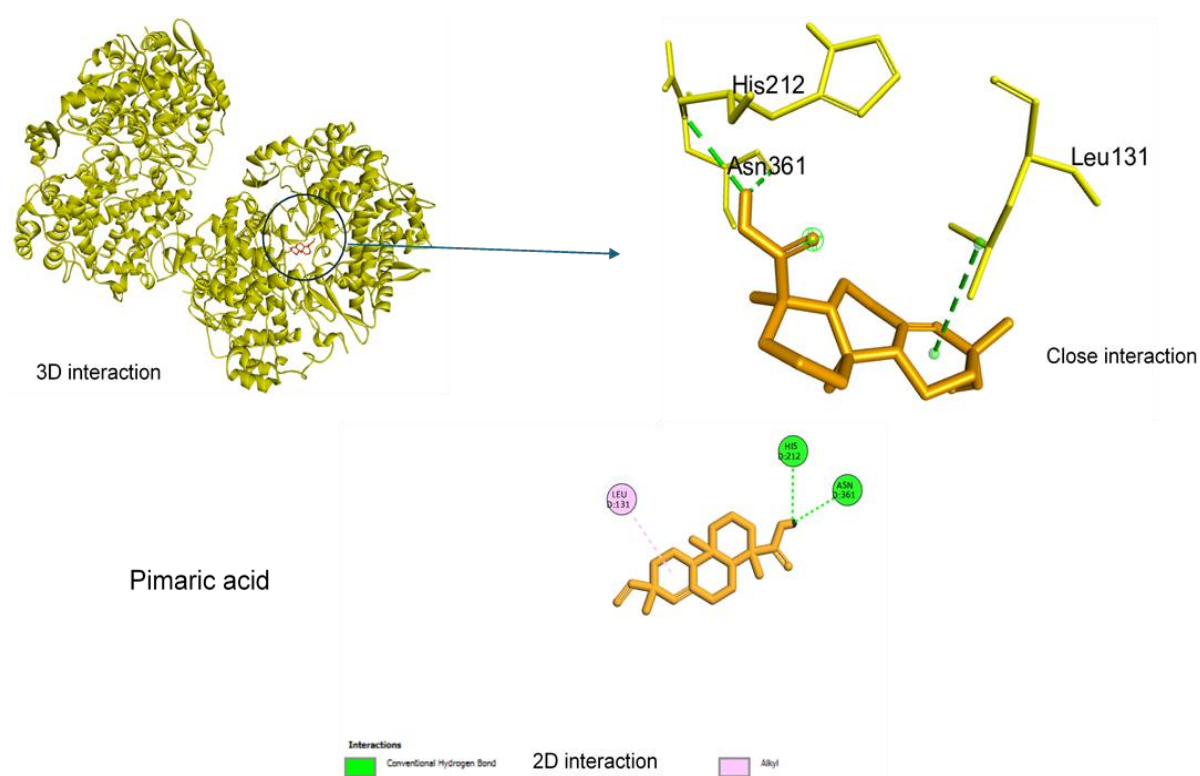


Figure S4. The docking poses of Pimaric with COX-2 and with interacted amino acids between ligand and COX-2 residues.

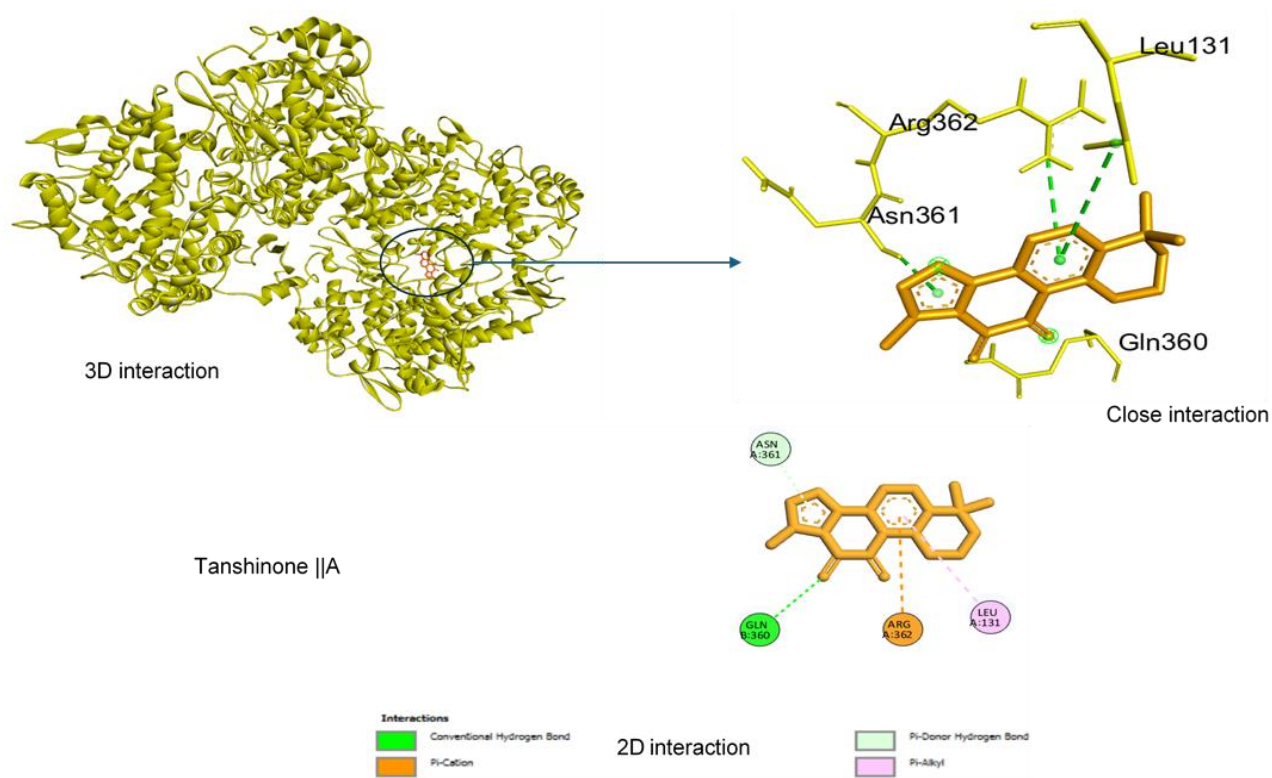


Figure S5. The docking poses of Tanshinone IIA with COX-2 and with interacted amino acids between ligand and COX-2 residues.

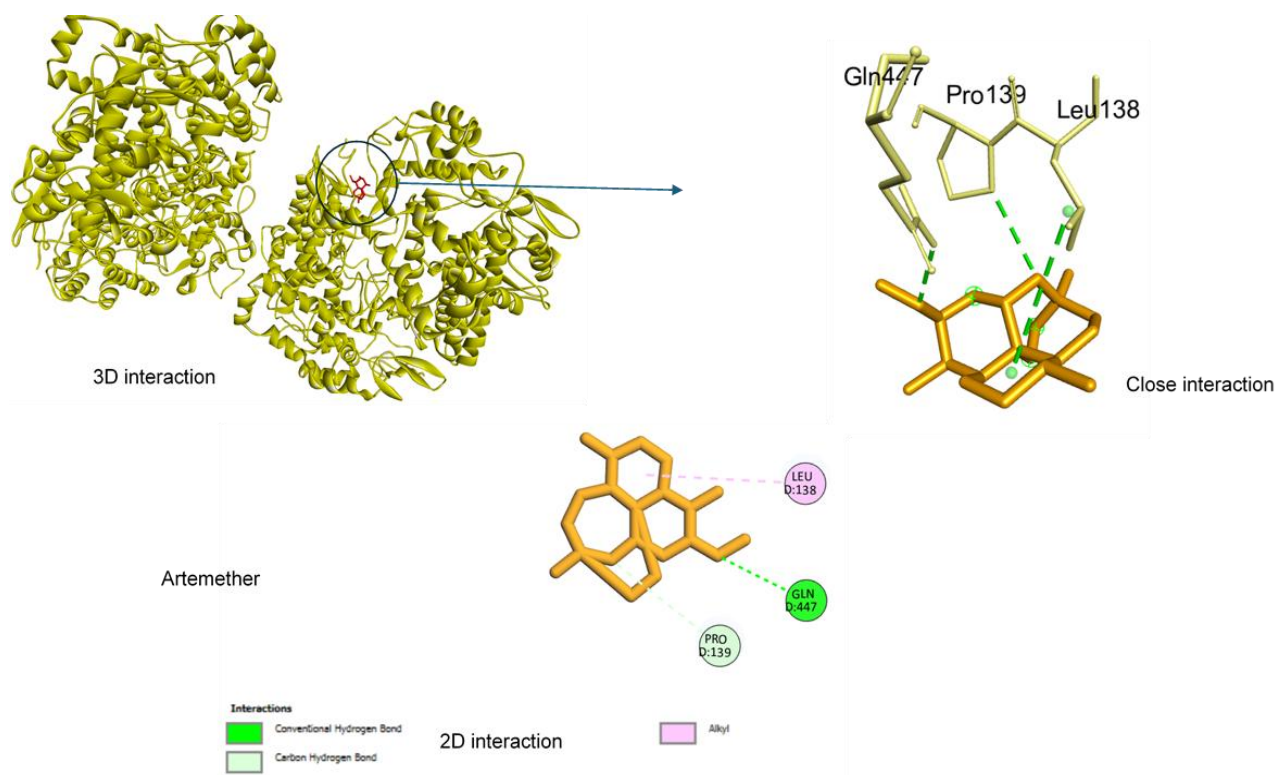


Figure S6. The docking poses of Artemether with COX-2 and with interacted amino acids between ligand and COX-2 residues.

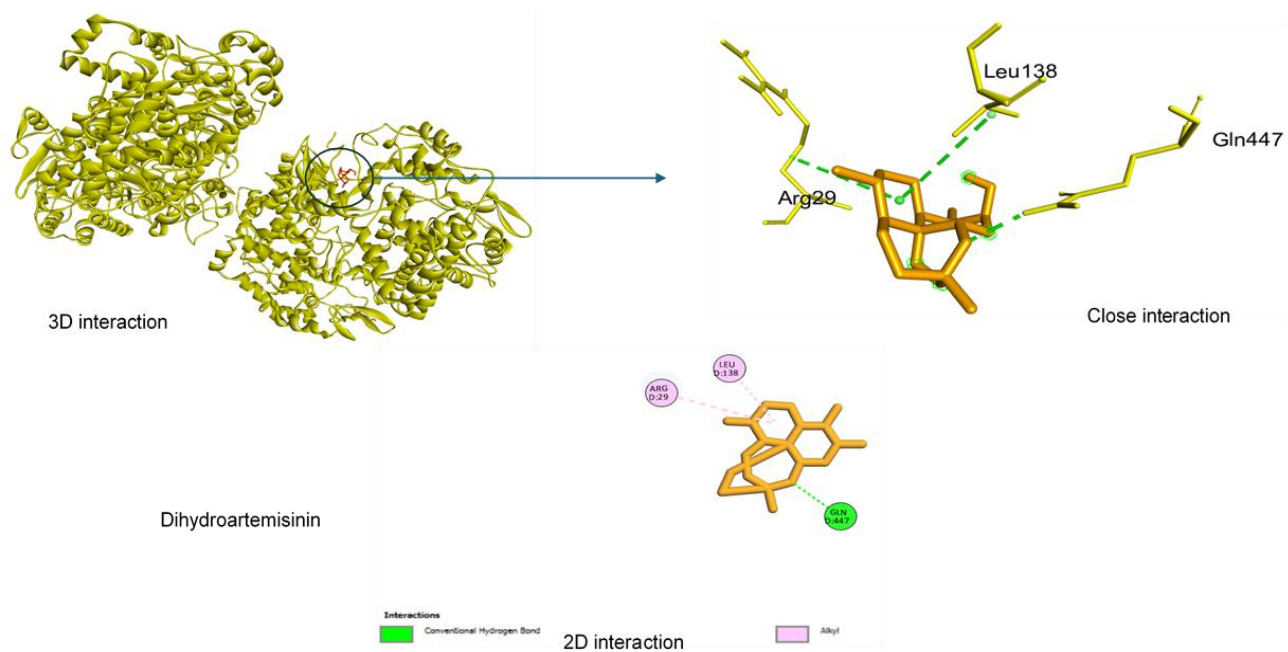


Figure S7. The docking poses of dihydroartemisinin with COX-2 and with interacted amino acids between ligand and COX-2 residues.

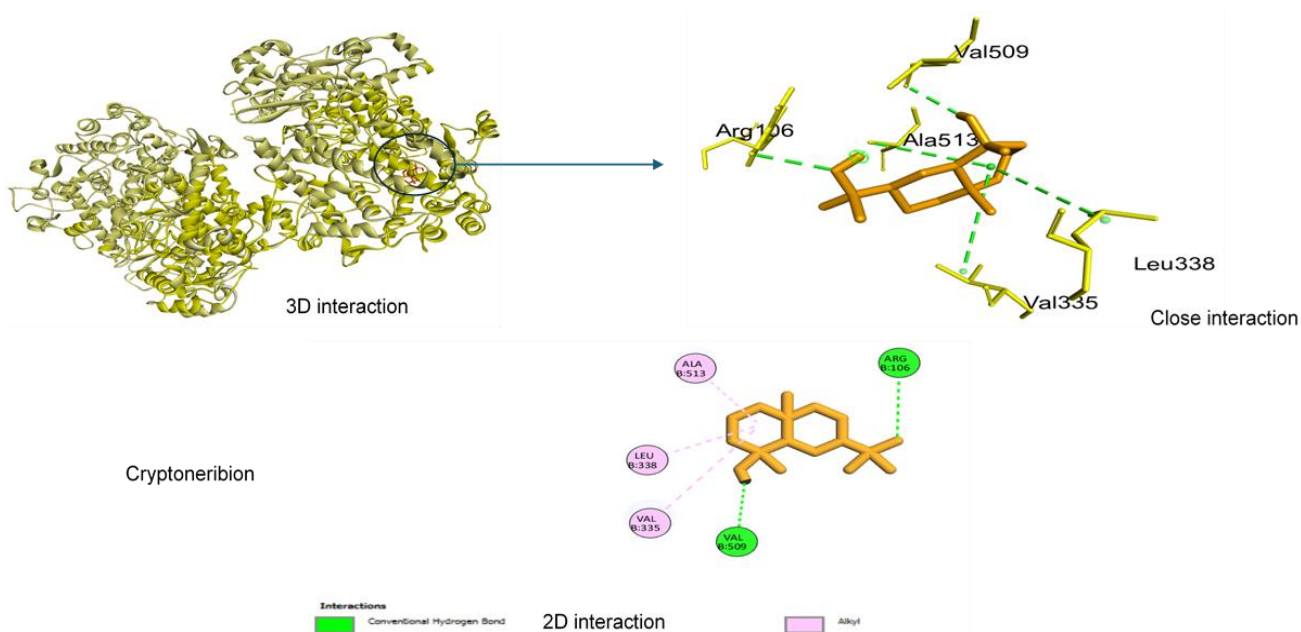


Figure S8. The docking poses of Cryptoneribion with COX-2 and with interacted amino acids between ligand and COX-2 residues.

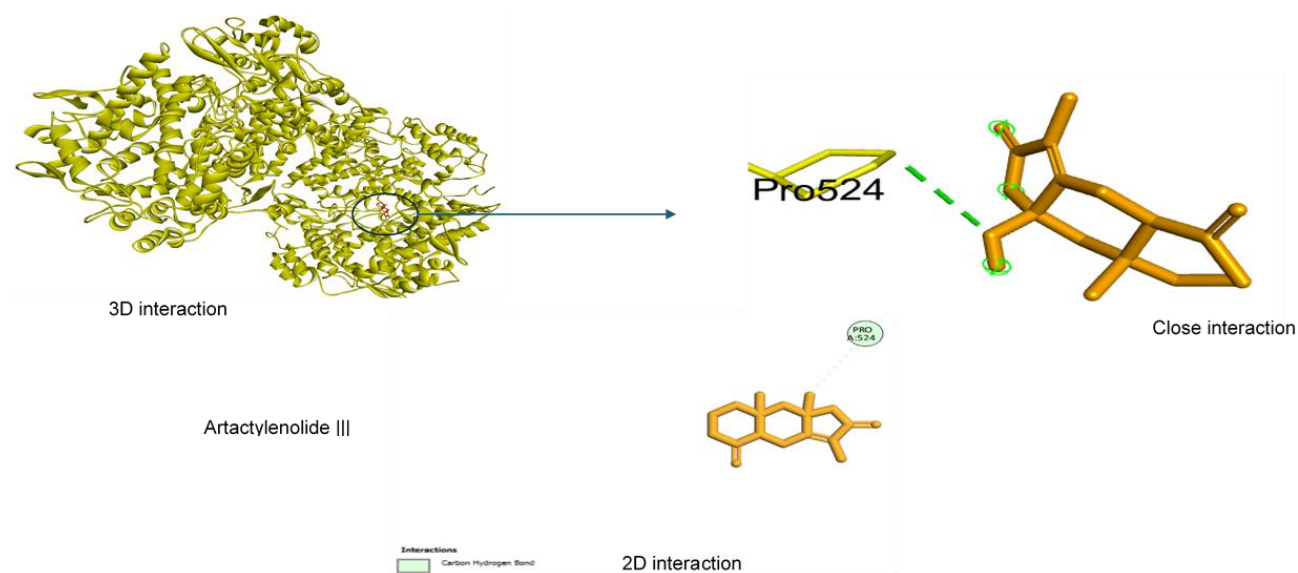


Figure S9. The docking poses of Artactylenolide III with COX-2 and with interacted amino acids between ligand and COX-2 residues.

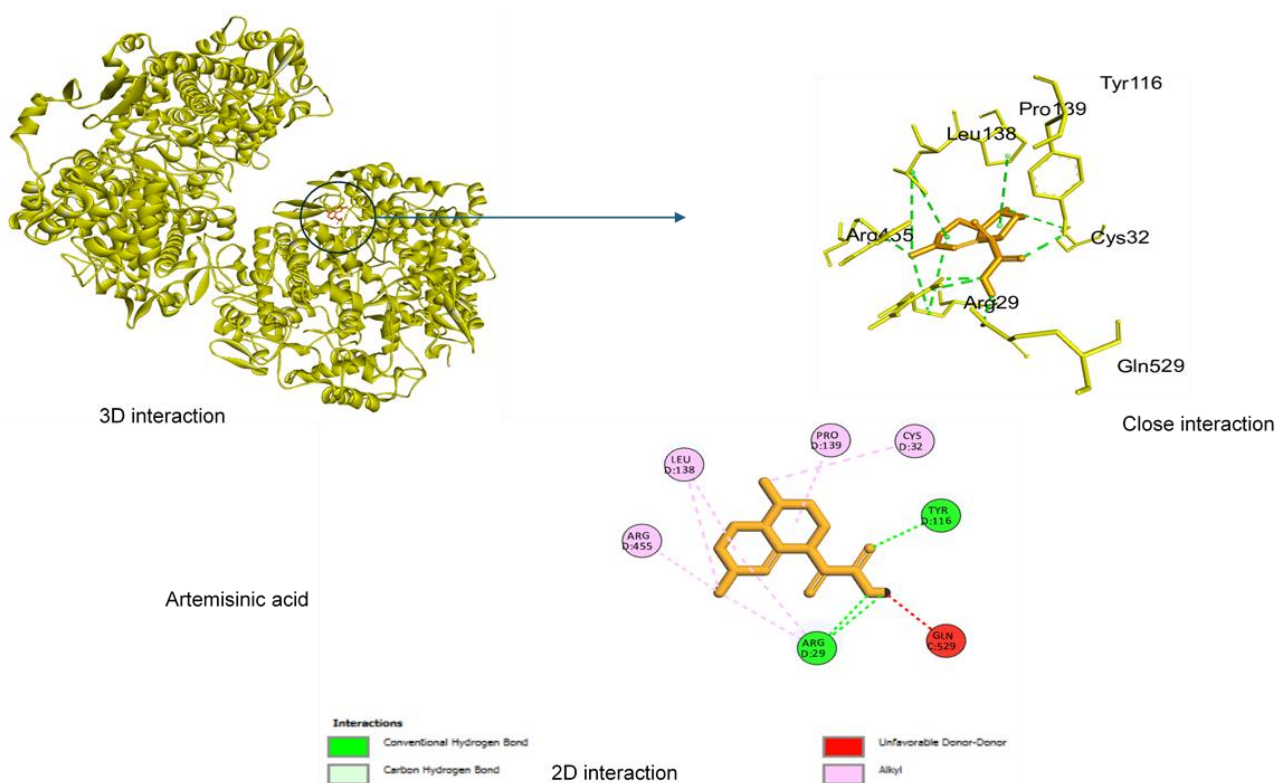


Figure S10. The docking poses of Artemisinic acid with COX-2 and with interacted amino acids between ligand and COX-2 residues.

Table S1: All the compounds pubchem IDs and links screened for COX-2

Compounds	Pubchem ID	Pubchem Link
Lactucin	442266	https://pubchem.ncbi.nlm.nih.gov/#query=442266
Parthenolide	7251185	https://pubchem.ncbi.nlm.nih.gov/compound/7251185
Dehydrocostuslactone	73174	https://pubchem.ncbi.nlm.nih.gov/compound/73174
Hyperoside	5281643	https://pubchem.ncbi.nlm.nih.gov/compound/5281643
Tanshinone I	114917	https://pubchem.ncbi.nlm.nih.gov/compound/114917
Artemisinic acid	10922465	https://pubchem.ncbi.nlm.nih.gov/compound/10922465
Artemether	68911	https://pubchem.ncbi.nlm.nih.gov/compound/68911
Arteether	3000469	https://pubchem.ncbi.nlm.nih.gov/compound/3000469
Dihydroartemisinin	3000518	https://pubchem.ncbi.nlm.nih.gov/compound/3000518
Artesunate	6917864	https://pubchem.ncbi.nlm.nih.gov/compound/6917864
Parviflorin	10100032	https://pubchem.ncbi.nlm.nih.gov/compound/10100032
Dehydrocostus lactone	73174	https://pubchem.ncbi.nlm.nih.gov/compound/73174
Tanshinone II	164676	https://pubchem.ncbi.nlm.nih.gov/compound/164676
Artemether methyl ester	36903603	https://pubmed.ncbi.nlm.nih.gov/36903603
Tanshinone II methyl ester	21476213	https://pubmed.ncbi.nlm.nih.gov/21476213
alpha-Eudesmol	92762	https://pubchem.ncbi.nlm.nih.gov/compound/92762
β-Eudesmol	91457	https://pubchem.ncbi.nlm.nih.gov/compound/91457
Chamazulene	10719	https://pubchem.ncbi.nlm.nih.gov/compound/10719
Guaiol	227829	https://pubchem.ncbi.nlm.nih.gov/compound/227829
Isocaryophyllene	5281522	https://pubchem.ncbi.nlm.nih.gov/compound/5281522
Costunolide	5281437	https://pubchem.ncbi.nlm.nih.gov/compound/5281437
Eudesmin	234823	https://pubchem.ncbi.nlm.nih.gov/compound/234823
Absinthin	442138	https://pubchem.ncbi.nlm.nih.gov/compound/442138
Anabsinthin	44558930	https://pubchem.ncbi.nlm.nih.gov/compound/44558930
Artemisin	65030	https://pubchem.ncbi.nlm.nih.gov/compound/65030
Artemisinin	68827	https://pubchem.ncbi.nlm.nih.gov/compound/68827
Alantactone	72724	https://pubchem.ncbi.nlm.nih.gov/compound/72724
Guaianolide A	53328018	https://pubchem.ncbi.nlm.nih.gov/compound/53328018
isosecotanapartholidea	13918473	https://pubchem.ncbi.nlm.nih.gov/compound/13918473
tanaphallin		https://pubmed.ncbi.nlm.nih.gov/23860275
8-hydroxy-3-methoxyisosecotanapartholide	102226846	https://pubchem.ncbi.nlm.nih.gov/compound/102226846
chrysartemin B	442147	https://pubchem.ncbi.nlm.nih.gov/compound/442147
Parthenin	442288	https://pubchem.ncbi.nlm.nih.gov/compound/442288
Hysterin	14165782	https://pubchem.ncbi.nlm.nih.gov/compound/14165782
Ambrosanolide	442306	https://pubchem.ncbi.nlm.nih.gov/compound/442306
Tetraneurin A	174868	https://pubchem.ncbi.nlm.nih.gov/compound/174868
Tetraneurin E	442306	https://pubchem.ncbi.nlm.nih.gov/compound/442306
Helenin	72724	https://pubchem.ncbi.nlm.nih.gov/compound/72724
Tetraneurin D	579318	https://pubchem.ncbi.nlm.nih.gov/compound/579318
Confertdiolide	101316900	https://pubchem.ncbi.nlm.nih.gov/compound/101316900
Eremophilene	12309744	https://pubchem.ncbi.nlm.nih.gov/compound/12309744
Pimaric acid	220338	https://pubchem.ncbi.nlm.nih.gov/compound/220338
Isopimaric acid	442048	https://pubchem.ncbi.nlm.nih.gov/compound/442048
Sugiol	94162	https://pubchem.ncbi.nlm.nih.gov/compound/94162
Cryptomeridiol	165258	https://pubchem.ncbi.nlm.nih.gov/compound/165258
santonin	221071	https://pubchem.ncbi.nlm.nih.gov/compound/221071
arsantin	10999985	https://pubchem.ncbi.nlm.nih.gov/compound/10999985
Costunolide	5281437	https://pubchem.ncbi.nlm.nih.gov/compound/5281437
dehydroleucodine	73440	https://pubchem.ncbi.nlm.nih.gov/compound/73440
Dehydrocostus lactone	73174	https://pubchem.ncbi.nlm.nih.gov/compound/73174
Atractylenolide I	5321018	https://pubchem.ncbi.nlm.nih.gov/compound/5321018
Atractylenolide II	14448070	https://pubchem.ncbi.nlm.nih.gov/compound/14448070
Atractylenolide III	155948	https://pubchem.ncbi.nlm.nih.gov/compound/155948
cumambrin A	174867	https://pubchem.ncbi.nlm.nih.gov/compound/174867
Artemisinic Acid	10922465	https://pubchem.ncbi.nlm.nih.gov/compound/10922465
cumambrin b	9992975	https://pubchem.ncbi.nlm.nih.gov/compound/9992975
Eupalinolide A	71463992	https://pubchem.ncbi.nlm.nih.gov/compound/71463992
Eupalinolide B	164885944	https://pubchem.ncbi.nlm.nih.gov/compound/164885944
EUPALINILIDE C	11417523	https://pubchem.ncbi.nlm.nih.gov/compound/11417523
EUPALINILIDE d	11347578	https://pubchem.ncbi.nlm.nih.gov/compound/11347578
EUPALINILIDE E	11188671	https://pubchem.ncbi.nlm.nih.gov/compound/11188671
EUPALINILIDE F	11429323	https://pubchem.ncbi.nlm.nih.gov/compound/11429323
EUPALINILIDE G	11474825	https://pubchem.ncbi.nlm.nih.gov/compound/11474825
Eupalinilide H	11361957	https://pubchem.ncbi.nlm.nih.gov/compound/11361957
EUPALINILIDE I	11292780	https://pubchem.ncbi.nlm.nih.gov/compound/11292780
Eupalinilide J	11328460	https://pubchem.ncbi.nlm.nih.gov/compound/11328460
Eupalinolide K	77985613	https://pubchem.ncbi.nlm.nih.gov/compound/77985613
Eupalinolide O	154809464	https://pubchem.ncbi.nlm.nih.gov/compound/154809464
Eupatolide	5281460	https://pubchem.ncbi.nlm.nih.gov/compound/5281460
artesanate	6917864	https://pubchem.ncbi.nlm.nih.gov/compound/6917864
Ainsliaside C	11969975	https://pubchem.ncbi.nlm.nih.gov/compound/11969975
Ainsliaside D	15071446	https://pubchem.ncbi.nlm.nih.gov/compound/15071446