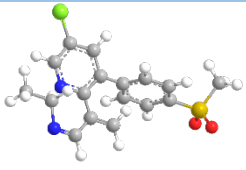
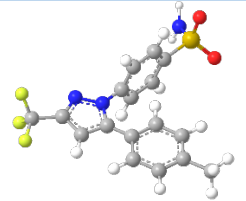
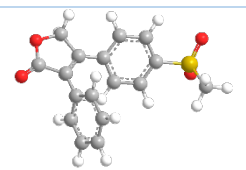
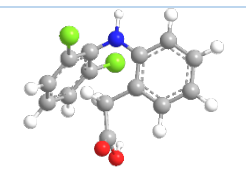
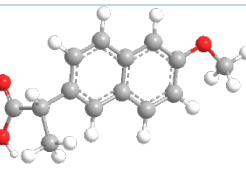
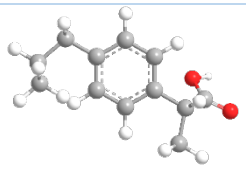


Computational Comparison of the Binding Affinity of Selective and Non-Selective NSAIDs to COX-2 Using Molecular Docking

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Drug	Structure	Union Free Energy (kcal/mol)	Inhibition Constant Ki (μM)
Etoricoxib		-11.22	0.006
Celecoxib		-10.89	0.0105
Rofecoxib		-10.23	0.0314
Diclofenac		-8.08	1.19
Naproxen		-7.29	4.50
Ibuprofen		-6.83	9.87

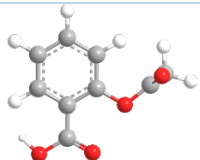
ASA		-4.56	452.07
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Table S1: Values of Free Energy of Binding and Inhibition Constant for COX-2 Selective and Non-Selective NSAIDs.

AutoDock 4		AutoDock Vina	
Group	Union Free Energy (kcal/mol)	Group	Union Free Energy (kcal/mol)
Selective NSAIDs	-10.78 ± 0.50	Selective NSAIDs	-8.5 ± 0.50
Non-Selective NSAIDs	-6.69 ± 1.51	Non-Selective NSAIDs	-7.45 ± 0.66

Table S2: Average Free Binding Energy of Selective and Non-selective NSAIDs according to AutoDock4 and AutoDock Vina.

Non-Selective Interaction Graphs

Diclofenac

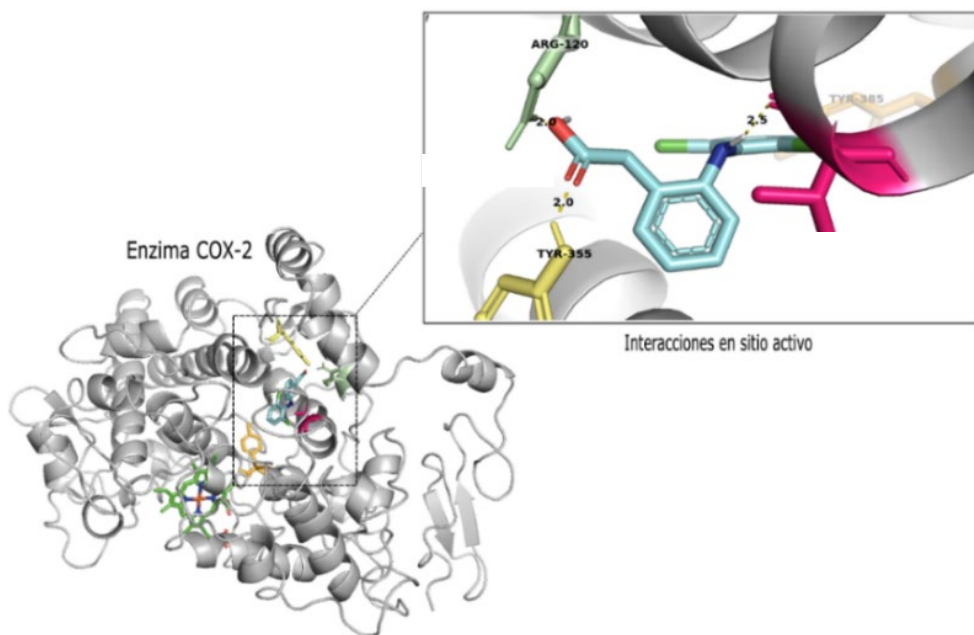


Figure S1. 3D Visualization of Hydrogen Bridges between Diclofenac and COX-2 at the Active Site.

Naproxen

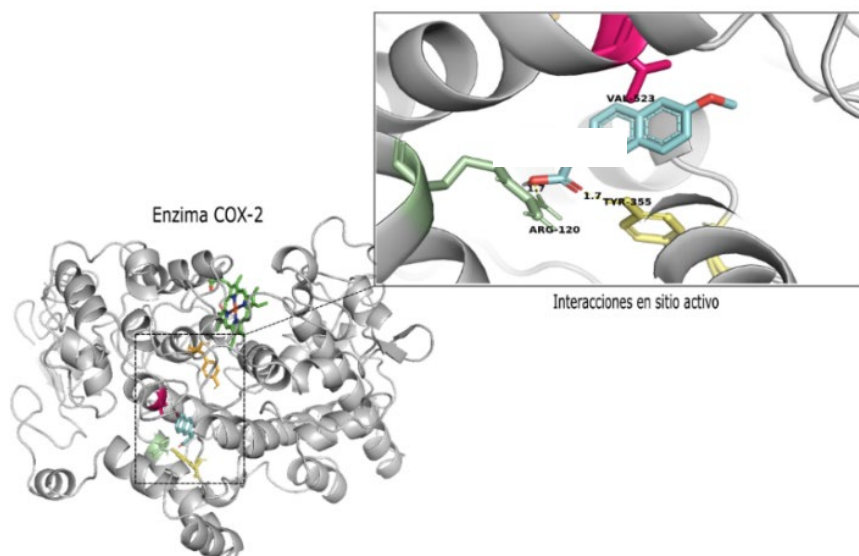


Figure S2. 3D Visualization of Hydrogen Bridges between Naproxen and COX-2 at the Active Site.

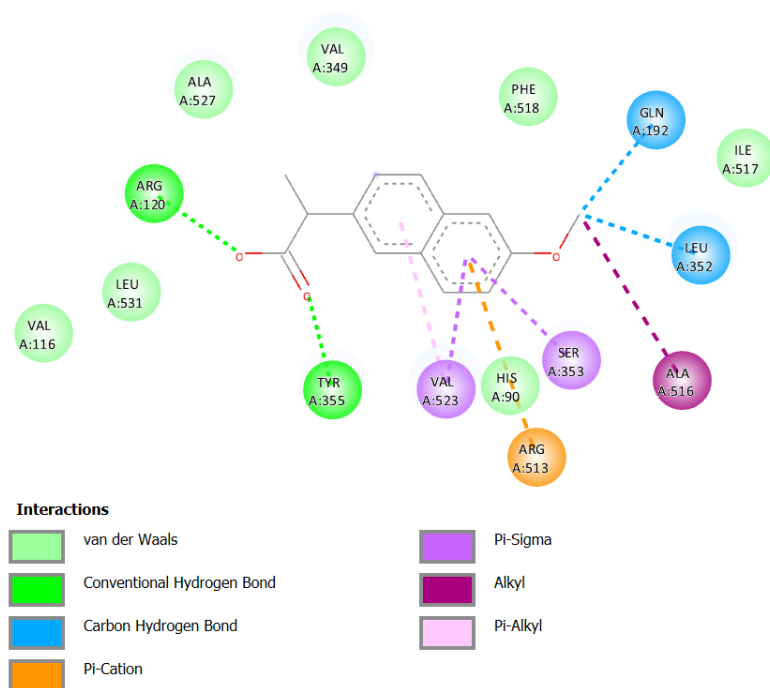


Figure S3. 2D Visualization of Hydrogen Bridges between Naproxen and COX-2 at the Active Site.

Ibuprofen

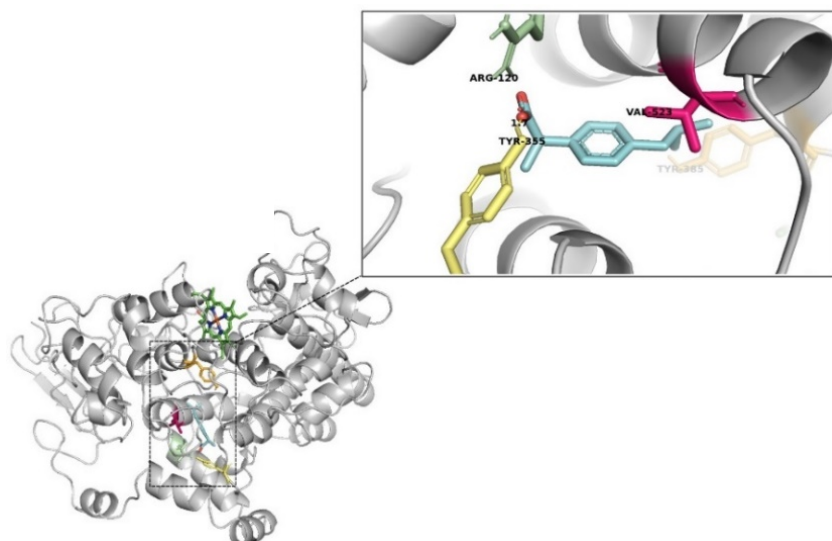


Figure S4. 3D Visualization of Hydrogen Bridges between Ibuprofen and COX-2 at the Active Site.

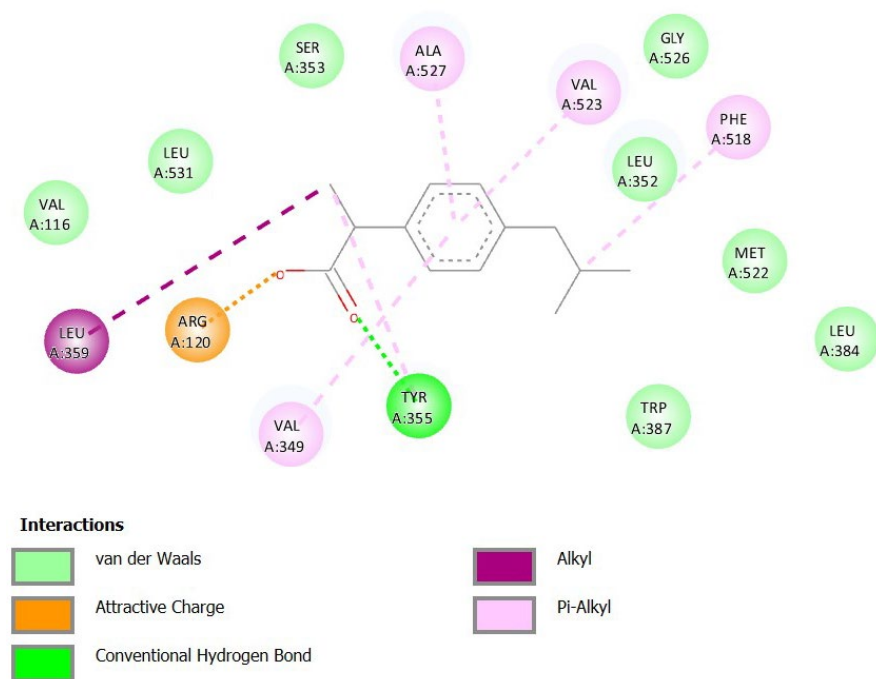


Figure S5. 2D Visualization of Hydrogen Bridges between Ibuprofen and COX-2 at the Active Site.

ASA

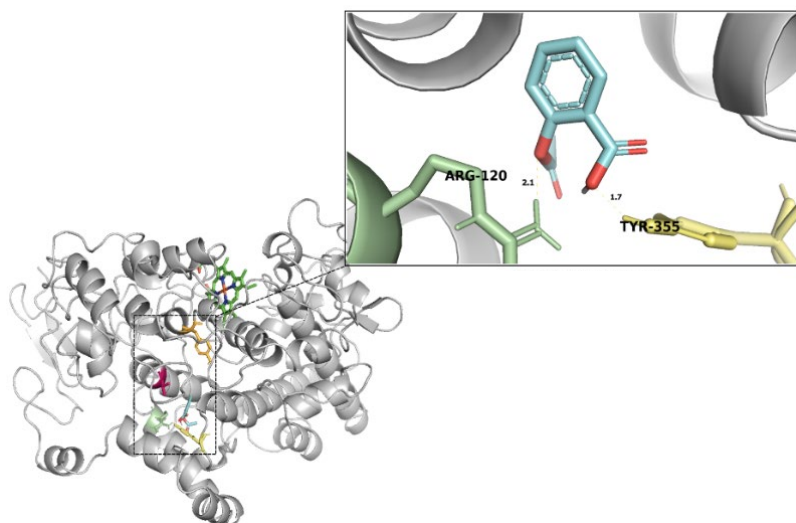


Figure S6. 3D Visualization of Hydrogen Bridges between ASA and COX-2 at the Active Site.

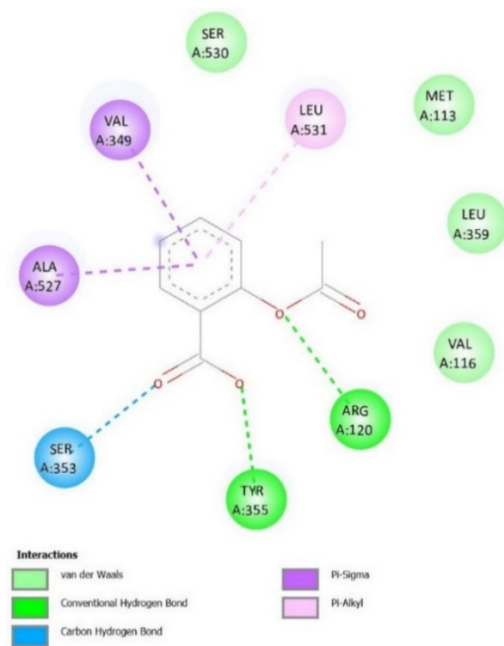


Figure S7. 2D Visualization of Hydrogen Bridges between ASA and COX-2 at the Active Site.

Selective Interaction Graphs

Etoricoxib

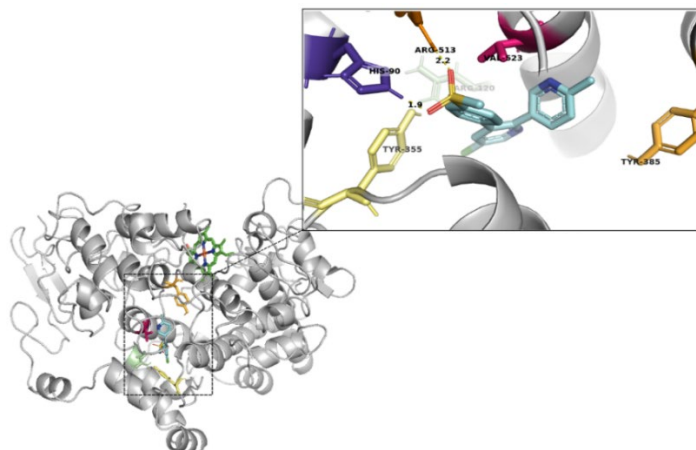


Figure S8. 3D Visualization of Hydrogen Bridges between Etoricoxib and COX-2 at the Active Site.

Celecoxib

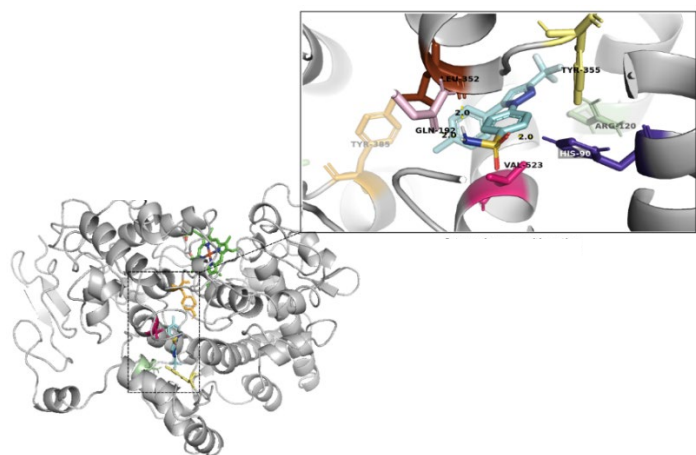


Figure S9. 3D Visualization of Hydrogen Bridges between Celecoxib and COX-2 at the Active Site.

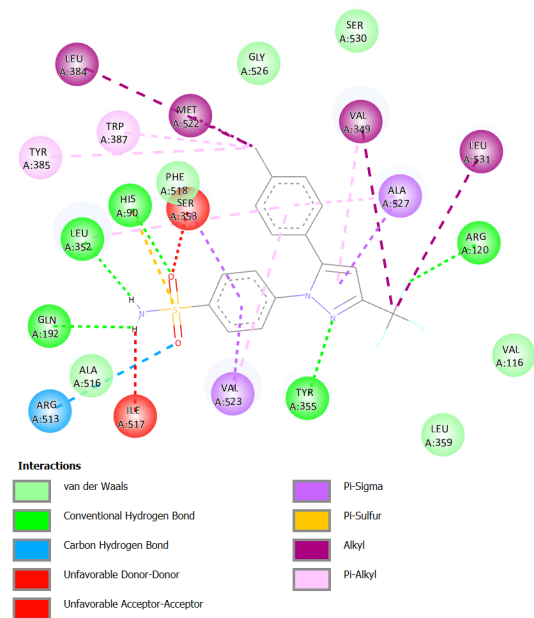


Figure S10. 2D Visualization of Hydrogen Bridges between Celecoxib and

COX-2 at the Active Site.

Rofecoxib

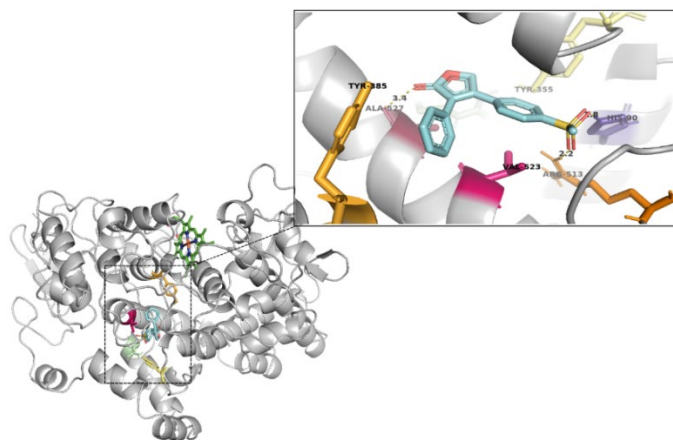


Figure S11. 3D Visualization of Hydrogen Bridges between Rofecoxib and COX-2 at the Active Site.

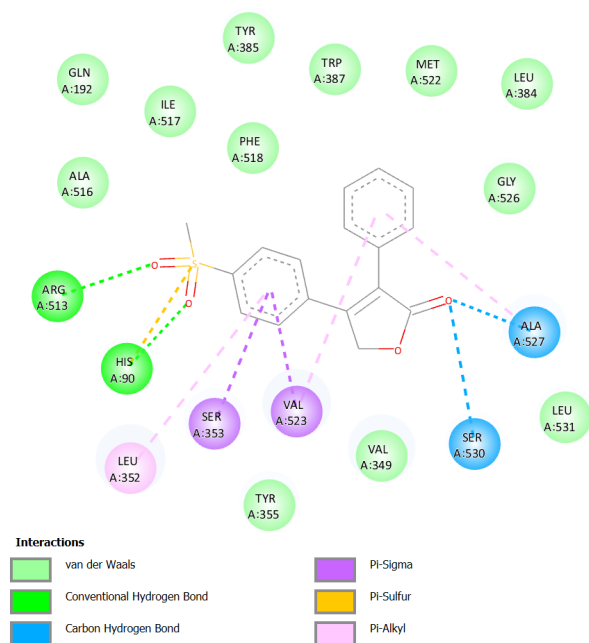


Figure S12. 2D Visualization of Hydrogen Bridges between Rofecoxib and COX-2 at the Active Site.