

Table S1. Proteins Used for Structure Determination Of 5-LOX

S.No	Protein I.D	Chain	E Value
1	2fnq	B	8.99e-146
2	2fnq	A	8.99e-146
3	2pom	A	4.78e-138
4	2pom	B	4.78e-138
5	1lox	A	3.72e-135
6	1hv9	A	1.64e-48
7	1jnj	A	1.64e-48
8	1n8q	A	1.64e-48
9	1no3	A	1.67e-48
10	1rrh	A	1.67e-48
11	1rrl	A	1.67e-48
12	1rrl	A	1.67e-48
13	1ik3	A	3.69e-48
14	1lnh	A	3.69e-48
15	2iuj	A	1.96e-46
16	1rov	A	2.85e-45
17	1iuk	B	2.65e-42
18	2sbl	A	7.59e-40
19	2sbl	B	7.59e-40
20	2sbl	A	7.59e-40
21	1f8n	A	1.44e-38
22	1yge	A	1.49e-38
23	1fgq	A	5.91e-38
24	1fgr	A	6.94e-38
25	1y4k	A	8.12e-38
26	1fgm	A	9.43e-38
27	1fgt	A	1.0e-37
28	1fgo	A	1.25e-37

Table S2. Observed Activity and Binding Energies of 1-PTH (COX-1 Pdb File) for Both Test and Training Set

Compound No.	Binding Energy (Kcals/mol)	Observed Activity (-log IC ₅₀)
1	-35.0697	-1.5119
3	-39.7176	-1.3729
5	-42.5336	-1.1139
6	-19.7704	-1.7750
7	-35.0481	-1.3222
8	-43.3761	-1.1139
9	-34.9397	-1.3444
10	-31.5364	-1.6646
11	-40.6763	-0.9547
13	-28.7564	-1.7832
15	-21.7176	-1.8149
16	-42.1629	-1.6031
17	-26.0979	-1.7589
2	-34.0704	-1.3729
4	-40.4583	-1.0253
12	-41.337	-1.7774
14	-23.8837	-1.9069

Table S3. Observed Activity and Binding Energies of 1-CX2 (COX-2 Pdb File) for Both Test and Training Set

Compound No.	Binding Energy (Kcals/mol)	Observed Activity (-log IC ₅₀)
1	-31.6164	-1.4579
3	-46.9846	-1.0792
5	-50.889	-0.7177
6	-48.453	-1.0792
8	-40.0408	-1.2648
9	-47.6887	-1.0492
11	-50.1963	-0.5315
12	-31.817	-1.4265
13	-41.0126	-1.1367
14	-31.8287	-1.4624
15	-56.158	-0.2765
16	-37.9511	-1.3692
17	-42.6751	-1.1492
2	-52.3918	-0.8716
4	-41.6667	-0.9547
7	-51.4392	-0.8987
10	-46.6514	-0.9552

Table S4. Observed Activity and Binding Energies of 5-LOX (Homology Model) for Both Test and Training Set

Compound No.	Binding Energy (Kcals/mol)	Observed Activity (-log IC ₅₀)
1	-43.5151	-0.9101
2	-38.8343	-1.1303
3	-44.6936	-1.1399
4	-39.2472	-1
5	-41.0613	-0.8808
6	-40.9602	-1.0792
7	-39.8223	-1.1271
8	-40.1173	-1
9	-42.5904	-1.0864
11	-45.6356	-0.6812
12	-46.5518	-0.7709
15	-54.1563	0.4318
16	-47.8358	-0.8136
10	-43.0525	-0.9777
13	-46.1833	-1.1461
14	-44.601	-1.1072
17	-45.6572	-0.8762