Supplementary Materials: Synthesis, Bioevaluation and Molecular Dynamic Simulation Studies of Dexibuprofen–Antioxidant Mutual Prodrugs

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Table S1. Chemo-informatics and biological properties of pro-drugs.

Properties	5a	5b	5c
Molecular formula	$C_{25}H_{38}O_4$	$C_{22}H_{24}O_6$	$C_{24}H_{24}O_6$
Mol. wt. (g/mol)	402.28	384.16	408.16
No. of HBA	4	6	6
No. of HBD	0	0	0
Log*P*	6.40	4.77	4.48
Polar surface area (PSA) (Å^2)	40.80	58.27	61.56
Molar refractivity (cm^3)	116.26	102.69	110.04
Density (g/cm^3)	1.03	1.20	1.21
Surface tension (dyne/cm)	38.3	46.4	48.1
Polarizability (cm^3)	46.08	40.71	43.62
Molecular volume (Å^3)	434.97	384.82	420.59
Drug score	0.83	1.22	1.04
Lipinski rule validation	Yes	Yes	Yes

Table S2. The binding energy values of all docked complexes.

Docking Poses	Ligand Binding	rmsd/ub	rmsd/lb
5a.1	−8.9	0	0
5a.2	−8.1	3.286	2.031
5a.3	−7.9	10.507	3.82
5a.4	−7.7	5.816	3.182
5a.5	−7.6	39.83	36.351
5a.6	−7.5	33.837	30.689
5a.7	−7.5	33.489	30.54
5a.8	−7.4	17.198	12.403
5a.9	−7.2	7.212	4.224
5b.1	−9.9	0	0
5b.2	−9.4	2.62	1.45
5b.3	−8.8	10.171	3.072
5b.4	−8.8	33.575	31.883
5b.5	−8.6	10.531	3.546
5b.6	−8.5	29.318	27.418
5b.7	−8.4	29.293	27.533
5b.8	−8.4	8.035	4.775
5b.9	−8.2	32.024	30.507
5c.1	−9.4	0	0
5c.2	−9.2	4.899	3.577
5c.3	−9.1	6.712	4.028
5c.4	−8.8	5.662	4.427
5c.5	−8.6	32.869	29.096
5c.6	−8.6	29.864	27.537
5c.7	−8.6	9.727	3.118
5c.8	−8.5	2.278	1.445
5c.9	−8.5	9.933	2.601

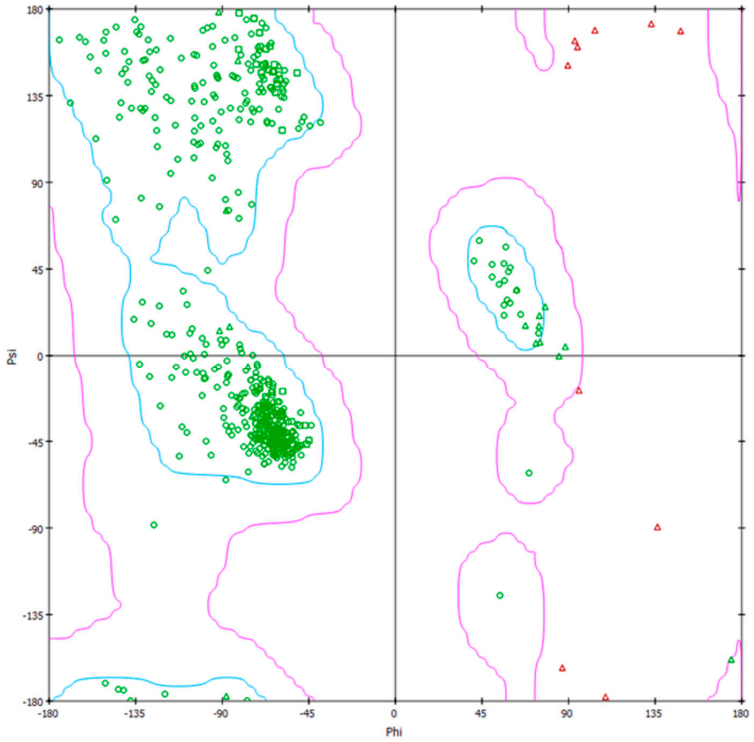

Figure S1. Ramachandran graph of target protein cycooxygenase-2, green (residues in favourable region), red (residues in allowed region).