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Supplementary material:

Table 1: Flavonoids and selective COX-2 blocker having anticancer activities.

Flavonoids	Pubchem id	Organ or tissue type	References
Delphinidin	CID 128853	Skin cancer	**[84, 85]**
Quercetin	CID 5280343	Skin cancer	**[86, 87]**
Myricetin	CID 5281672	Skin cancer	**[88-92]**
Equol	CID 91469	Skin cancer, Prostate cancer, Breast Cancer	**[93, 94]**
Isorhamnetin	CID 5281654	**Article I.** Skin cancer, Colon cancer, Colorectal cancer	**[95-97]**
Quercetin-3-methyl ether	CID 5280681	**Article II.** Skin cancer, Breast cancer, Leukaemia	**[98-100]**
Kaempferol	CID 5280863	Skin cancer, Colon cancer	**[101-103]**
Eriodictyol	CID 440735	Skin cancer, Breast Cancer	**[104, 105]**
Luteolin	CID 5280445	Skin cancer, Lung cancer, Prostate cancer, Colon cancer.	**[106-110]**
5-deoxykaempferol	CID 5281611	Skin cancer	**[111]**
7,3',4'-Trihydroxyisoflavone	CID 5284648	Skin cancer	**[72]**
4',6,7-trihydroxyisoflavone	CID 5284649	Colon cancer	**[112]**
Celocoxib	CID 2662	Cyclooxygenase-2 inhibitor in cancer	**[113, 114]**

Table 2: Summary of FlexX docking results with COX-2 and ligands.

Flavonoids	Score	Match	Lipo	Ambig	Clash	Rot	ΔG Kj/mol	Ligand Efficiency
Celocoxib	-26.85	-21.15	-14.73	-7.33	6.77	4.2	-29	0.27
Isorhamnetin	-20.93	-22.32	-11.21	-8.56	8.76	7.0	-30	0.31
5-deoxykaempferol	-19.26	-15.65	-11.83	-5.77	4.40	4.2	-29	0.35
Equol	-21.94	-17.43	-12.88	-5.71	4.48	4.2	-27	0.36
4',6,7-trihydroxyisoflavone	-20.61	-17.03	-10.03	-6.17	3.89	4.2	-26	0.31
Eriodictyol	-24.63	-24.97	-11.21	-7.43	6.58	7.0	-23	0.26
Quercetin	-21.66	-24.06	-11.19	-6.85	8.05	7.0	-20	0.21
Myricetin	-21.59	-23.18	-12.27	-7.26	7.38	8.4	-19	0.20
7,3',4'-Trihydroxyisoflavone	-26.25	-23.85	-11.82	-6.92	6.75	4.2	-18	0.22
Quercetin-3-methyl ether	-24.88	-25.55	-10.48	-7.76	6.51	7.0	-16	0.16
Kaempferol	-20.92	-17.93	-13.00	-7.33	6.35	5.6	-15	0.17
Delphinidin	-18.41	-23.92	-11.55	-7.36	10.36	8.4	-15	0.16
Luteolin	-27.67	-26.93	-10.23	-7.25	5.75	5.6	-13	0.14

Table 3: Type of interactions and interacting amino acid residues of COX-2 protein with selected ligands, generated from ArgusLab.

Flavonoids	Binding Energy kcal/mol	H-Bonding	Hydrophobic Bonding			Pi-Cation
			Pi - Alkyl	Pi-Pi	Pi-Sigma	
Celecoxib	-9.35	Q^{192}, R^{120}, L^{531},S^{530}	V^{523},A^{527},L^{352}, F^{198}	-	V^{349}, Y^{348}	-
Isorhamnetin	-8.25	-	V^{349}, L^{352}, V^{523}.	-	S^{353},A^{527}, V^{523}	-
5-deoxykaempferol	-9.14	-	V^{523}, I^{517}, A^{516}	Y^{355}	V^{349}	-
Equol	-9.92	Q^{192}, F^{518}	V^{523}, V^{349}, L^{352},L^{531},A^{527}	-	-	-
4',6,7-trihydroxyisoflavone	-9.89	S^{530}	V^{523}, A^{527}, L^{352}, L^{531}	-	V^{349}	-
Eriodictyol	-9.50	F^{518}, R^{120}	-	-	A^{527}, V^{349}, V^{523}	-
Quercetin	-8.94	R^{513}, R^{120}, Q^{192}	V^{523}, V^{349}, L^{352}	-	V^{523}, A^{527}	-
Myricetin	-8.91	R^{120}	V^{349}, V^{523}	-	A^{527}, V^{523}	-
7,3',4'-Trihydroxyisoflavone	-9.86	-	A^{527}, V^{523}, L^{531}, L^{352}	-	S^{353}, V^{349}	-
Quercetin-3-methyl ether	-8.26	H^{90}, S^{530}	A^{527}, V^{349}, L^{352}	-	V^{349}, V^{523}	-
Kaempferol	-10.64	W^{385}, S^{530}	V^{349}, L^{352}	-	L^{352}, V^{523}, A^{516}	
Delphinidin	-8.94	E^{524}	V^{89}, V^{116}, I^{112}	Y^{355}	L^{93}	R^{120}
Luteolin	-10.72	S^{530}	A^{516}, L^{352}, V^{349}	-	V^{523}	-