

Supplementary material:

Table 1: Table representing amino acids contributing for binding pocket and chemo-preventive analysis for the top 9 anti-angiogenic natural compounds screened through HEX.

Serial no	Molecule (Compound Id)	Amino acid base (H bond distance in Å ⁰)	Ames test	Health effect						rank
				Blood	Cardiovascular system	Gastrointestinal system	Kidney	Liver	Lungs	
1	Pazopanib (P)	LEU 32 (1.63), GLY 59 (1.73)	0.048	0.57	0.75	0.93	0.27	0.23	0.50	Ref
2	Lactoferrin (L)	GLU 30 (2.21), PRO 28 (2.57), HIS 27 (2.03)	0.642	0.93	0.99	1.00	0.93	0.98	0.99	-
3	Benzophenone 3 (Be)	LEU 32 (2.77), GLY 52 (2.03)	0.099	0.11	0.29	0.28	0.33	0.04	0.55	-
4	Phytoestrogens (Ph)	GLY 59 (2.71)	0.105	0.31	0.41	0.30	0.87	0.49	0.40	-
5	Finasteride (F)	LEU 32 (1.56), GLY 59 (2.17)	0.001	0.82	0.91	0.65	0.92	0.94	0.98	4
6	Curcumin (C)	PHE 47 (2.01)	0.033	0.62	0.95	0.24	0.42	0.69	0.51	1
7	Epigallocatechin Gallate [EGCG] (E)	GLU 13 (1.21)	0.037	0.78	0.92	0.98	0.83	0.67	0.96	2
8	Milk Thistle (M)	GLY 59 (2.22)	0.262	0.99	0.93	1.00	0.87	0.90	0.95	-
9	Npfl-86i (N)	LEU 32 (2.44), CYS 32 (2.46), THR 31 (2.34)	0.237	0.77	0.97	1.00	0.73	0.98	0.99	-
10	Barringtonol (B)	GLU 30 (2.50), 1.59)	0.000	0.80	1.00	0.99	1.00	0.77	1.00	3

	GOOD		MODERATE		POOR		REFERENCE
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