

SUPPORTING INFORMATION

Active Phytochemicals of Indian Spices Target Leading Proteins Involved in Breast Cancer: An in Silico Study

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Table S1. Molecular Docking interaction of all phytochemicals with BCL3 and CXCL10. For a better view, the docking interaction of phytochemicals and proteins are amplified from protein-phytochemical complexes

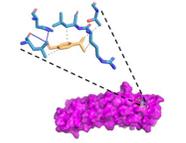
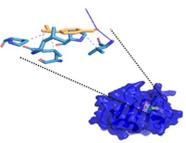
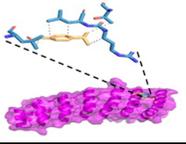
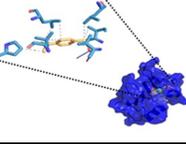
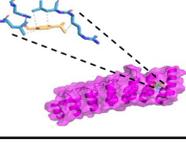
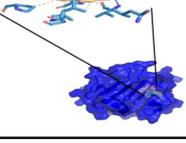
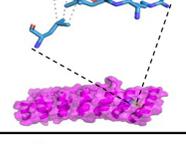
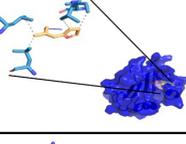
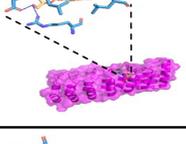
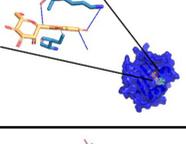
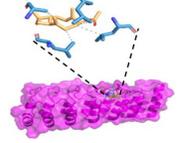
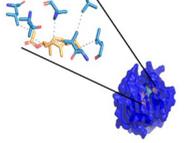
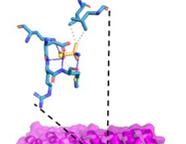
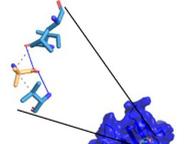
S. No.	Indian Spices (botanical names)	Compounds	PubChem ID	Docking interactions with BCL3	Binding energy (kcal mol ⁻¹)	Binding constant (×10 ³) mol ⁻¹	Docking interactions with CXCL10	Binding energy (kcal mol ⁻¹)	Binding constant (×10 ³) mol ⁻¹
1	Cumin (<i>Cuminum cyminum</i>)	4-isopropylbenzyl alcohol	CID_325		-4.9	3.52		-5.3	6.85
		4-isopropyl phenyl acetaldehyde	CID_61359		-5.1	4.91		-5.6	11.3
		4-isopropylbenzaldehyde	CID_326		-5.1	4.91		-5.6	8.1
2	Cinnamon (<i>Cinnamomum verum</i>)	2-methyl-3-(2-furyl) propenal	CID_6210220		-4	0.785		-4.7	2.52
3	Clove (<i>Syzygium cyminum</i>)	Isobiflorin	CID_85114699		-6.1	26.02		-6.6	59.87
		Caryophyllenyl acetate	CID_91749980		-5.6	11.3		-6.7	70.73
4	Fenugreek (<i>Trigonella foenum graecum</i>)	2-aminoisobutyric acid	CID_6119		-3.8	0.56		-3.8	563.03

Table S1. Molecular Docking interaction of all phytochemicals with BCL3 and CXCL10. For a better view, the docking interaction of phytochemicals and proteins are amplified from protein-phytochemical complexes

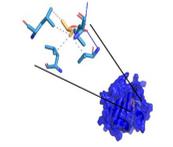
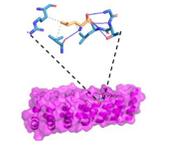
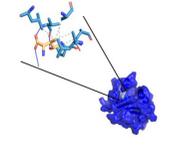
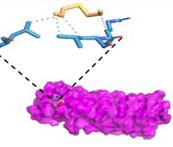
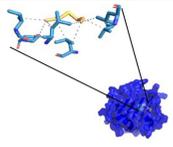
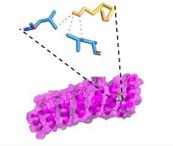
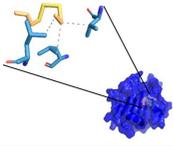
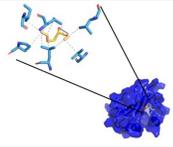
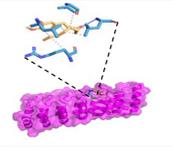
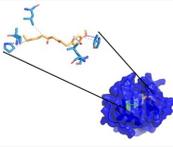
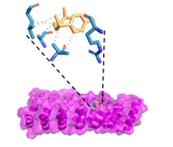
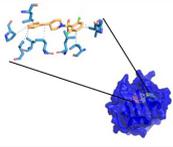
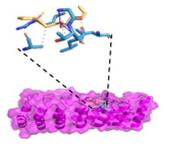
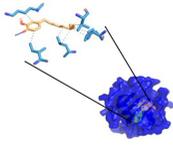
4	Fenugreek (<i>Trigonella foenum graecum</i>)	Furaneol	CID_19309		-4.2	1.09		-4.6	2.13
		Hydroxyisoleucine	CID_6918732		-4.5	1.8		-4.6	2.13
5	Garlic (<i>Allium sativum</i>)	Diallyl sulphide	CID_11617		-2.9	0.125		-3.3	0.24
		Diallyl trisulfide	CID_16315		-2.8	0.1		-3.2	0.2
		Allicin	CID_65036		-3.6	0.4		-3.7	0.47
6	Ginger (<i>Zingiber officinale</i>)	Gingerol	CID_442793		-5	4.16		-6	22.02
		Zingiberene	CID_92776		-4.8	2.98		-6.4	42.9
		6-Shogaol	CID_11152		-5.3	6.85		-6	22.02

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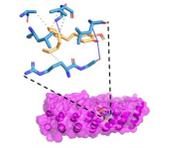
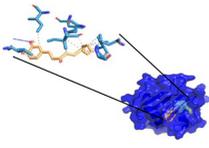
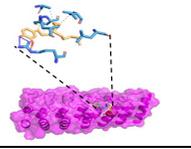
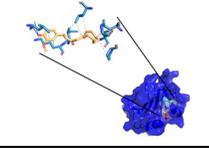
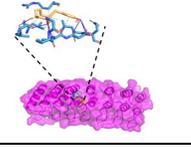
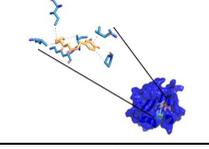
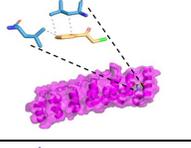
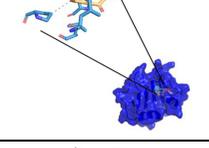
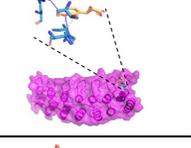
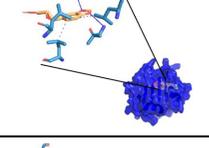
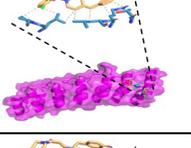
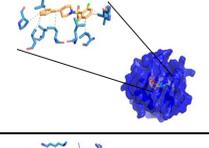
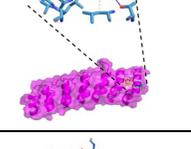
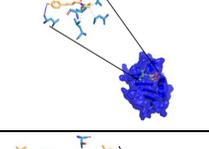
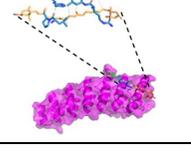
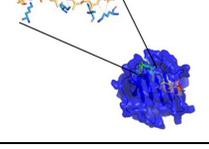
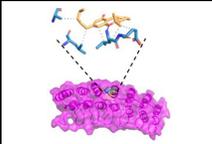
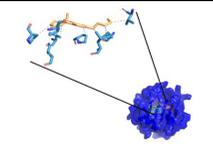
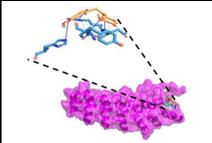
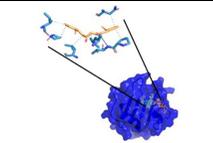
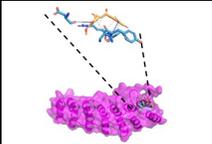
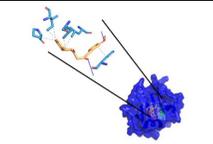
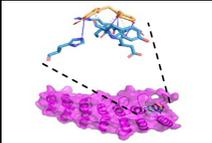
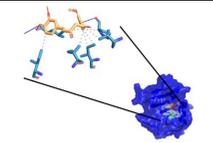
6	Ginger (<i>Zingiber officinale</i>)	8-Shogaol	CID_6442560		-5.1	4.91		-6.1	26.02
		10-Shogaol	CID_6442612		-4.9	3.52		-6	22.02
		Gingerdiol	CID_11369949		-5.6	11.3		-5.7	13.35
7	Nutmeg (<i>Myristica indicum</i>)	2-chloroacetophenone	CID_72864		-4.7	2.52		-5.1	4.91
8	Pepper (<i>Piper nigrum</i>)	Fraxidin	CID_3083616		-5.1	4.91		-5.5	9.57
		Piperidine	CID_8082		-6.3	36.31		-7.4	227.14
		Coumaperine	CID_10131321		-6.2	30.74		-6.4	42.9
9	Red chilli (<i>Capsicum annuum</i>)	Capsanthin	CID_5281228		-7.2	162.75		-7.7	374.49

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10	Sesame (<i>Sesamum indicum</i>)	Dronabinol	CID_16078		-5.8	15.78		-7.4	227.14
11	Turmeric (<i>Curcuma longa</i>)	Diferuloylmethane	CID_969516		-5.7	13.35		-6.8	83.56
		Curcumin	CID_969516		-5.6	11.3		-6.5	50.68
		Curcumin D6	CID_53464495		-5.8	15.78		-6.3	36.31