

Screening of phytochemicals for potential breast cancer targets BRCA1 and BARD1: A network pharmacology approach

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Supplementary Data

Table S1 — Information of the target proteins -BRCA1 and BARD1.

Protein	PDB ID	Active sites	Function
Breast Cancer Type 1 Susceptibility Protein (BRCA1)	IJM7	I21, L22, G23, P25, I31, I42, L63, F79	Repairing DNA double strand break
Brcal-Associated Ring Domain Protein 1 (BARD1)	IJM7	K46, L47, L48, R49, C50, L57, G67, H68, I69, L101	Control of the cell cycle in response to DNA damage

Table S2 — Grid box coordinates and size parameters of the protein target BRCA1 and BRAD1

Protein		Coordinates		
		x	y	z
BRCA1	Center (Å)	7.68	-1.918	5.982
	Box Size (Å)	50	40	48
BRAD1	Center (Å)	-7.448	-4.626	-3.096
	Box Size (Å)	40	48	46

Table S3 — Drug likeliness properties of the top scoring phytochemicals.

Phytochemicals	Lipinski	Pfizer	GSK	GoldenTriangle
Maclurin	Accepted	Accepted	Accepted	Accepted
6-thioguanosine 5'-diphosphate	Rejected	Accepted	Rejected	Accepted
6-Biopterin	Accepted	Accepted	Accepted	Accepted
Gallocatechin	Accepted	Accepted	Accepted	Accepted
Paeonidin-3-5,-Diglucoiside	Rejected	Accepted	Rejected	Rejected
Anthraquinones Emodin	Accepted	Accepted	Accepted	Accepted
Clavatul	Accepted	Accepted	Accepted	Rejected
2'-Deoxycytidine	Accepted	Accepted	Accepted	Accepted
Adenine	Accepted	Accepted	Accepted	Rejected
(+)-Scytalone	Accepted	Accepted	Accepted	Rejected
Plantamajoside	Rejected	Accepted	Rejected	Rejected
3,4-dihydroxyphenyl	Rejected	Accepted	Rejected	Rejected
Myoinositol	Accepted	Accepted	Accepted	Rejected
L-(+)-Quercitol	Accepted	Accepted	Accepted	Rejected
Leucoanthocyanidin	Accepted	Accepted	Accepted	Accepted
D-Glucosamine	Accepted	Accepted	Accepted	Rejected
Okanin	Accepted	Accepted	Accepted	Accepted
Neoisostilbin	Rejected	Accepted	Rejected	Accepted
Acteoside	Rejected	Accepted	Rejected	Rejected

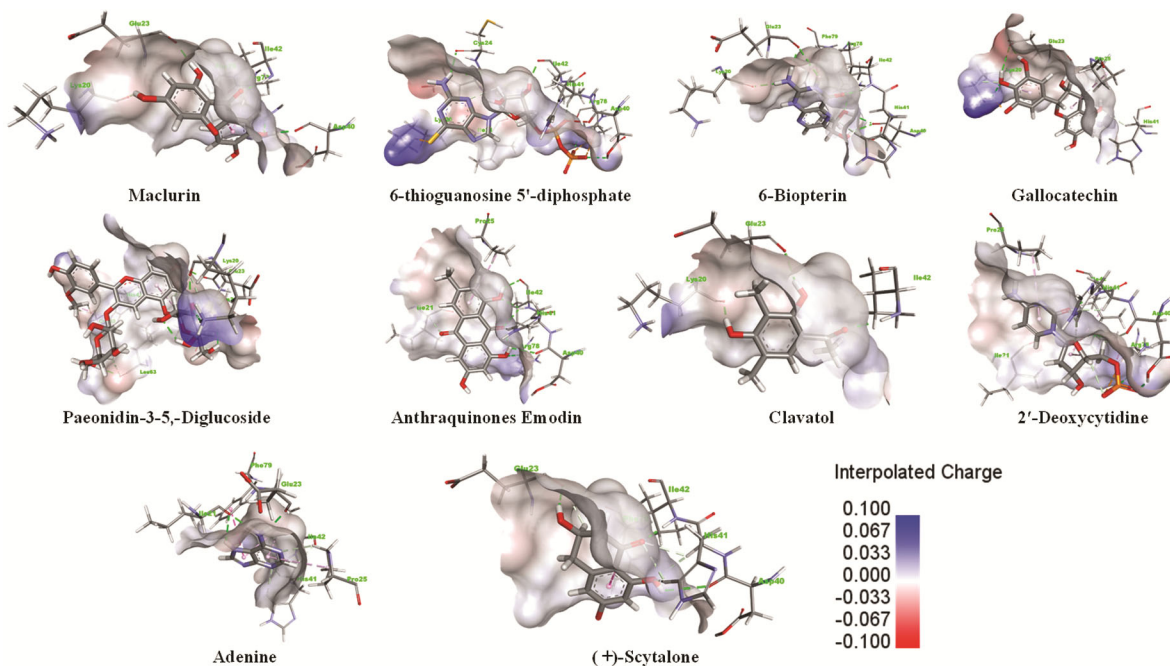


Fig. S1 — Electrostatic interaction diagram of BRCA1 protein target with top 10 phytochemicals individually which was generated using Discovery Studio tool.

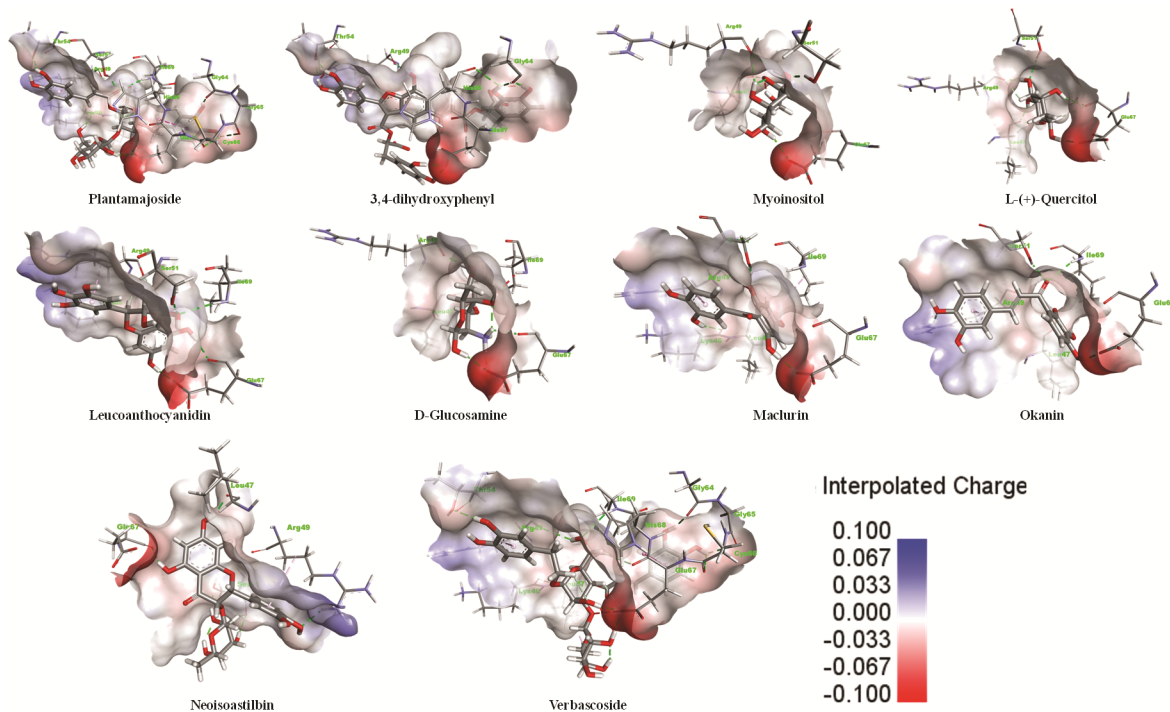


Fig. S2 — Electrostatic interaction diagram of BRAD1 protein target with top 10 phytochemicals individually which was generated using Discovery Studio tool.