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.

<table>
<thead>
<tr>
<th>Protein</th>
<th>PDB ID</th>
<th>Active sites</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Breast Cancer Type 1 Susceptibility Protein (BRCA1)</td>
<td>IJM7</td>
<td>I21, L22, G23, P25, I31, I42, L63, F79</td>
<td>Repairing DNA double strand break</td>
</tr>
<tr>
<td>Brca1-Associated Ring Domain Protein 1 (BARD1)</td>
<td>IJM7</td>
<td>K46, L47, L48, R49, C50, L57, G67, H68, I69, L101</td>
<td>Control of the cell cycle in response to DNA damage</td>
</tr>
</tbody>
</table>

Table S2 — Grid box coordinates and size parameters of the protein target BRCA1 and BARD1

<table>
<thead>
<tr>
<th>Protein</th>
<th>Coordinates</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>BRCA1</td>
<td>Center (Å)</td>
<td>7.68</td>
<td>-1.918</td>
<td>5.982</td>
</tr>
<tr>
<td></td>
<td>Box Size (Å)</td>
<td>50</td>
<td>40</td>
<td>48</td>
</tr>
<tr>
<td>BRAD1</td>
<td>Center (Å)</td>
<td>-7.448</td>
<td>-4.626</td>
<td>-3.096</td>
</tr>
<tr>
<td></td>
<td>Box Size (Å)</td>
<td>40</td>
<td>48</td>
<td>46</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Phytochemicals</th>
<th>Lipinski</th>
<th>Pfizer</th>
<th>GSK</th>
<th>GoldenTriangle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maclurin</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
</tr>
<tr>
<td>6-thioguanosine 5'-diphosphate</td>
<td>Rejected</td>
<td>Accepted</td>
<td>Rejected</td>
<td>Accepted</td>
</tr>
<tr>
<td>6-Biopterin</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
</tr>
<tr>
<td>Galloolatechin</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
</tr>
<tr>
<td>Paeonidin-3,5-Diglucoside</td>
<td>Rejected</td>
<td>Accepted</td>
<td>Rejected</td>
<td>Rejected</td>
</tr>
<tr>
<td>Anthraquinones Emodin</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
</tr>
<tr>
<td>Clavatol</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Rejected</td>
</tr>
<tr>
<td>2′-Deoxyxycytidine</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
</tr>
<tr>
<td>Adenine</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Rejected</td>
</tr>
<tr>
<td>(+)-Scytalalone</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Rejected</td>
</tr>
<tr>
<td>Plantamajoside</td>
<td>Rejected</td>
<td>Accepted</td>
<td>Rejected</td>
<td>Rejected</td>
</tr>
<tr>
<td>3,4-dihydroxyphenyl</td>
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<td>Accepted</td>
<td>Rejected</td>
<td>Rejected</td>
</tr>
<tr>
<td>Myoinositol</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Rejected</td>
</tr>
<tr>
<td>L(+)-Quercitol</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Rejected</td>
</tr>
<tr>
<td>Leucoanthocyanidin</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Rejected</td>
</tr>
<tr>
<td>D-Glucosamine</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Rejected</td>
</tr>
<tr>
<td>Okamin</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
<td>Accepted</td>
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<tr>
<td>Neoisostilbin</td>
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<td>Accepted</td>
<td>Rejected</td>
<td>Accepted</td>
</tr>
<tr>
<td>Acteoside</td>
<td>Rejected</td>
<td>Accepted</td>
<td>Rejected</td>
<td>Rejected</td>
</tr>
</tbody>
</table>
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.