

## Supplementary Materials

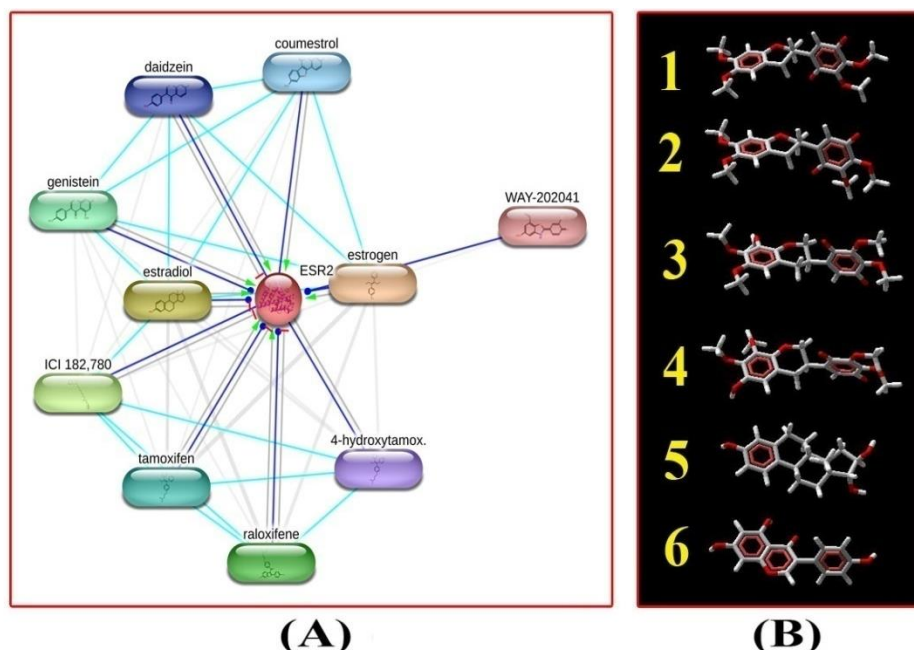
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# In Silico Computational Prediction of Anti-Breast Cancer Effect of Abruquinones from *Abrus precatorius* L.

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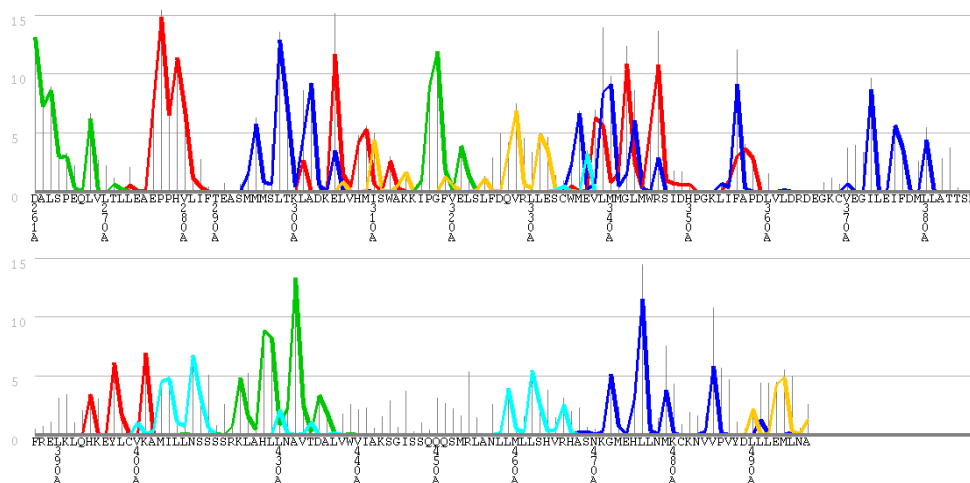
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### STITCH 3.1 Output



**Figure S1.** Selection of candidate ligands. (A). Action view of the STITCH 3.1 results for the query estrogen receptor in *Homo sapiens*. This view summarizes the network of predicted associations for a particular group of proteins and chemicals. The action view was obtained with a medium confidence (0.400) level output to the 10 best-scoring hits. Green color indicates activation; Red color indicates inhibition; Blue color indicates binding. (B). Ligands PDB files processed by MVD: abruquinone (32) A (1), abruquinone (18) A (2), abruquinone B (3), abruquinone C (4), estriol (5) and genistein (6).

### GHECOM 1.0 server Output



**Figure S2.** Prediction of pocketnes by GHECOM 1.0 server. This program finds multi-scale pockets on the protein surfaces using mathematical morphology. The line shows the value of pocketnes [%] for each residue. A residue in a deeper and larger pocket has a larger value of pocketnes. The color of pocketnes bar indicates cluster number of pocket (red: cluster 1, blue: cluster 2, green: cluster 3, yellow: cluster 4, cyan: cluster 5, gray: other clusters).