

Supplementary Materials

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

Mijanur Rahman and Shahdat Hossain*

Laboratory of Alternative Medicine & Behavioral Neurosciences, Department of Biochemistry and Molecular Biology, Jahangirnagar University, Savar, Dhaka 1342, Bangladesh.

STITCH 3.1 Output

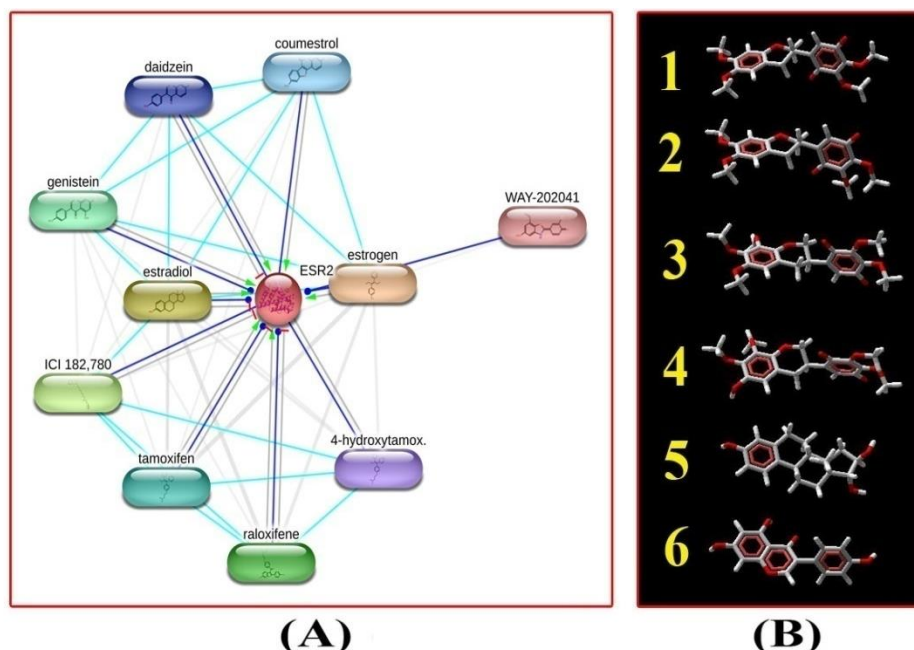


Figure S1. Selection of candidate ligands. (A). Action view of the STITCH 3.1 results for the query estrogen receptor in *Homo sapiens*. This view summarizes the network of predicted associations for a particular group of proteins and chemicals. The action view was obtained with a medium confidence (0.400) 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

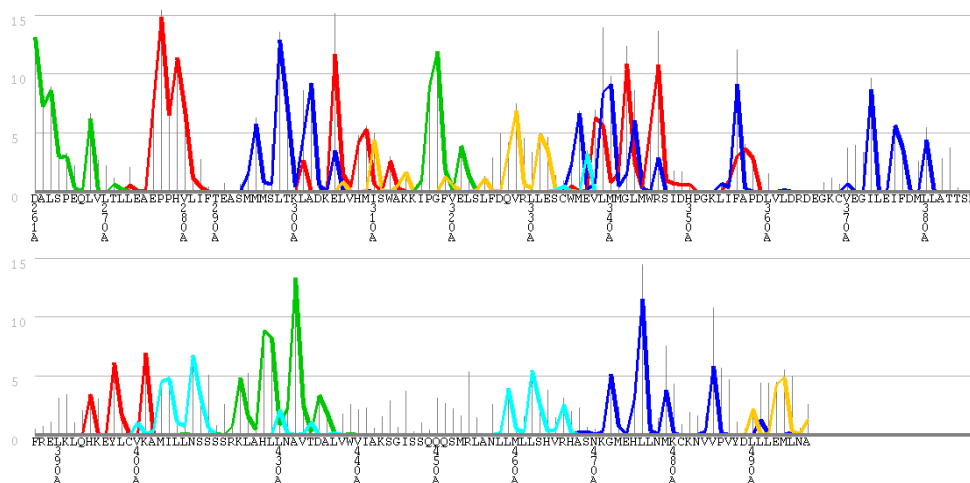


Figure S2. Prediction of pocketnes by GHECOM 1.0 server. This program finds multi-scale pockets on the protein surfaces using mathematical morphology. The line shows the value of pocketnes [%] for each residue. A residue in a deeper and larger pocket has a larger value of pocketnes. The color of pocketnes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