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