**Highlights**

* Kalanchoe pinnata phytochemicals studied to inhibit breast cancer.
* DFT, PASS, ADMET, Molecular Docking studied to filter ligands.
* Molecular Dynamic Simulation was employed to identify dynamic characteristics.
* MMPBSA and PCA studied to find better medication properties.
* Hit7 (Kaempferol) acted as a better drug candidate than D1 (Aredia).