

Title: In silico of *Jatropha Gossypifolia*-derived Compounds Against Breast Cancer Targeting PR, p130Cas and hER α using Molecular Docking, DFT, MM-GBSA, and Molecular Dynamics Simulations

Presenting Author Details:

Emmanuel Kitete Mulongo, University of Kinshasa, Kinshasa, D.R. Congo

Co-Authors:

K.N Nyiwa Ngbolua; P.T Mpiana, University of Kinshasa, Kinshasa, D.R. Congo



Abstract:

Breast cancer is one of those diseases that strikes the world regardless of continent. By the beginning of 2021, more than 7.8 million women had been diagnosed with breast cancer over five years, while in 2022, it caused 670,000 deaths globally. For this study, three receptors have been considered: the human progesterone receptor (PR), the human estrogen receptor alpha (hER α), and the Cas family scaffolding protein (p130Cas). 67 compounds identified in *Jatropha gossypifolia* have been used as ligands.

Nine compounds (Gadain, Apigenin, Cleomiscosin A, Jatrophone, Gossypifan, Falodone, Schaftoside, Isoschaftoside, and Citlalitrione) have exhibited significant activities after molecular docking with 3ERT, 4OAR, and 5W93, giving a lower binding energy ΔG than Paclitaxel, the control. The Molecular Dynamics Simulations at 200 ns revealed that Gossypifan and Gadain are binding better with 3ERT than other ligands, considering RMSF, Protein-ligand contacts, and ligand properties, while schaftoside and isoschaftoside are binding better with 5W93 than other ligands, considering RMSD, RMSF, Protein-ligand contacts, and ligand properties. The MM-GBSA with 3ERT shows Apigenin displays the strongest affinity, along with robust interactions and maximum effectiveness. Gossypifan provides a reasonable balance but features less effective interactions. Gadain falls short in all areas, especially regarding ligand effectiveness. In summary, Apigenin stands out as the most potent compound. With 5W93, the MM-GBSA shows Schaftoside exhibits the highest overall affinity, even with a solvation drawback. Isoschaftoside achieves a favorable balance between affinity and stability. In contrast, Isovitexin lacks adequate affinity, despite being structurally stable. In summary, Schaftoside stands out as the most effective compound in terms of affinity.

These results enlighten the potential of *Jatropha gossypifolia*. We are actually verifying this in vitro and in vivo.

Biography:

Emmanuel Kitete Mulongo is a Ph.D. student at the University of Kinshasa, Democratic Republic of the Congo. He holds a degree in Analytical Chemistry from the University of Kisangani. His research focuses on the valorization of medicinal plants native to the country, particularly through the evaluation of their preventive and therapeutic potential against various diseases.