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3D SRUCTURE-LIGAND BASED AND ADME PREDICTION OF α-MANGOSTIN AND ITS DERIVATIVES AGAINST ESTROGEN RECEPTOR α

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α-mangostin is the main active compound of *Garcinia mangostana* pericarp, which inhibits the proliferation of the MCF-7 cell line with an IC_{50} 20 μM. Molecular docking simulation and 3D structure-based pharmacophore models were employed to identify the molecular interactions of α-mangostin and its derivatives against estrogen receptor α (ERα). The results showed that the binding energy of α-mangostin and its best derivative (AMD10) were −9.05 kcal/mol and −11.89 kcal/mol, respectively. These compounds also interacted with Thr347, Asp351, Met388, Met528, Ile424, Arg394, and Glu353. The pharmacophore-fit scores of α-mangostin and AMD10 were 83.06% and 86.46%, respectively. In addition, the absorption, distribution, metabolism and excretion (ADME) properties were predicted. These results showed that α-mangostin and AMD10 are promising candidates of novel anti-breast-cancer agents with antagonistic activity to ERα.

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