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| **Related works on docking studies** | **Software’s/Tools used in the papers** | **References** |
| Identification the possible targets for anticancer agents | Auto Dock, GOLD and Glide | (Adeniyi et al., 2013) |
| Mdm2/Mdmx Inhibitor targets the identification of cancer | GOLD, Glide, MOE-dock and Auto Dock Vina | (Baratham et al., 2014) |
| Identification of novel chemical entities for multiple diseases | Glide, Auto Dock Vina, GLOD, Surflex-Dock, FlexX, ICM(Internal Coordinate Mechanic), and DOCK | (Perez et al., 2016) |
| Structure-Based Multi-targeted for breast cancer | Auto Dock Vina, MOE-dock, FlexX, and GOLD | (Acharya et al., 2019) |

Table S1: Comparative molecular docking studies focused on the evolution of docking programs