KIRTHIKA G M.Pharm (Pharmacology)

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Project: **Structure based design of RSK2 Inhibitors for Triple Negative Breast Cancer Therapy**

This project focused on identifying novel small-molecule inhibitors of **RSK2** as a therapeutic strategy for **Triple-Negative Breast Cancer (TNBC)**. Using a combined computational and in-vitro approach, focused compound libraries were virtually screened, followed by binding free-energy evaluation and molecular dynamics simulations.

Two shortlisted flavonoids—**Hesperetin and Diosmetin**—were experimentally validated for their antiproliferative, chemo-sensitizing, and anti-migratory effects in Gemcitabine-treated TNBC cells. Both compounds significantly enhanced Gemcitabine sensitivity and inhibited migration/invasion, indicating strong potential to overcome chemoresistance in aggressive TNBC.

SKILLS GAINED

Hard Skills

- Virtual screening and molecular docking
- Mammalian cell culture and aseptic techniques
- Antiproliferative, migration & invasion assays
- Preparation of drug solutions and laboratory reagent management
- Data analysis, interpretation, and scientific documentation

Soft Skills

- Independent project planning & execution

- Critical thinking and experimental troubleshooting
- Attention to detail and adherence to lab safety
- Scientific communication (reports, presentations)
- Problem-solving and adaptability in both computational and wet-lab environments