Research Plan TEMPLATE

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| **Student name:** |  |
| **Student email:** |  |
| **Degree program:** |  |
| **Advisor name:** |  |
| **Advisor email:** |  |
| **Date:** |  |

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| *By specifying the Problem statement and Data sources, instructors, advisors and others may thereby suggest projects via template for completion by the student.* |

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| **Credits [1-3]:** | 1 |

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| Problem statement | *The problem statement provides a clear and concise description of the issue that the project will address.* |

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| 4OH-Tamoxifen is a widely prescribed breast cancer drug, and known anti-estrogen, which binds Estrogen Receptor alpha (ERalpha), a nuclear receptor (NR), and GPR30, a G-protein coupled receptor (GPCR).   * From [PubChem](https://pubchem.ncbi.nlm.nih.gov/) and [DrugCentral](https://drugcentral.org/), find and download data on this drug, 4OH-Tamoxifen. * From the [NCBI Gene database](https://www.ncbi.nlm.nih.gov/gene/), search for GPR30 and download available data. * Search [RCSB Protein Data Bank (PDB)](https://www.rcsb.org/) for 3ERT (HUMAN ESTROGEN RECEPTOR ALPHA) and download the PDB and FASTA files. * Generate homology model for GPR30 using [T-COFFEE](http://tcoffee.crg.cat/). * Dock 4OH-Tamoxifen against models of (1) ERalpha and (2) GPR30, using AutoDock or OpenEye or other package. * Visualize the docked models of protein-ligand complexes; identify and analyze binding interactions.   Presentation of results should include graphical representations of binding, and analysis of the molecular interactions. The final report should be interpretable by pharmaceutical scientists concerned with drug discovery for disease areas related to these protein targets.  Alternatively, a different drug and different proteins may be used, with a pharmaceutical motivation. |

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| Data sources | *Source and dataset specification sufficient to facilitate verification of accessibility by the student for the project.* |

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| * Datasource: [NCBI Gene database](https://www.ncbi.nlm.nih.gov/gene/) * Datasource: [RCSB Protein Data Bank (PDB)](https://www.rcsb.org/) * Datasource: [PubChem](https://pubchem.ncbi.nlm.nih.gov/) * Datasource: [DrugCentral](https://drugcentral.org/) |

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| *Students must complete the elements of this template to comprise a preliminary research plan for instructor approval.* |

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| Title | *The title should be descriptive and comprehensible to the intended audience.* |

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| Topics; keywords | *Keywords for the relevant area[s] of biomedical data science.* |

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| Investigator roles and training | *Describe what role each person will play on the project team and what each person’s responsibility(ies) and deliverables will be. How has the investigator's coursework and other training prepared them for these roles?* |

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| Abstract | *Abstracts provide a comprehensive summary of the research project. For preliminary abstracts, it is understood that revisions may be required depending on results.* |

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| Introduction; overview | *Provide a brief description of the background needed to understand your project, and how it relates to biomedicine and data science.* |

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| Importance | *Why is your project problem important to biomedical science, medicine, public health or others? Cite relevant references if possible.* |

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| Objectives | *Provide a list of the specific answers, results, datasets, tools, and/or other deliverables that will be generated by completing the project.* |

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| Methodology | *Methodology defines the methods and logic steps that will be taken to solve the project problem and to achieve proposed objectives. Software should be specified, particularly any specialized scientific software tools.* |

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