Research Plan TEMPLATE

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

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

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

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

|  |
| --- |
| The overall task, in the context of early stage drug discovery, is to model the bioactivity of a dataset of lead candidate molecules against the receptor sites of the following proteins:   * ERα (estrogen receptor alpha) * ERγ (estrogen receptor gamma) * AR (androgen receptor)   Target Based Virtual Screening (TBVS) may be achieved via docking, using OpenEye Docking, or AutoDock, or other packages. For an example test set, use a list of molecules from PubChem that are similar to estradiol.  Ligand Based Virtual Screening (LBVS) typically involves similarity searching using a known active ligand. Numerous online, standalone, free and commercial packages are available.  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. |

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

|  |
| --- |
| * Datasource: [RCSB Protein Data Bank (PDB)](https://www.rcsb.org/) * Datasource: [PubChem](https://pubchem.ncbi.nlm.nih.gov/) * Datasource: [ZINC](https://zinc.docking.org/) |

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

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

|  |
| --- |
|  |

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

|  |
| --- |
|  |

|  |  |
| --- | --- |
| 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?* |

|  |
| --- |
|  |

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

|  |
| --- |
|  |

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

|  |
| --- |
|  |

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

|  |
| --- |
|  |

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

|  |
| --- |
|  |

|  |  |
| --- | --- |
| 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.* |

|  |
| --- |
|  |