I. Disclaimer:

1. The following materials only cover the fundamental knowledge required for this project, not necessarily comprehensive.
2. We are not responsible for any potential data lost or hardware damage for using the software recommended here.
3. We have tried our best to ensure that the links provided here are safe but it's the user's responsibility to be cautious when using the links.

II. Question-guided materials for self-study

Handouts (docx) on basic biochem, links to software download page or web services, and links to (hopefully) mobile-friendly recommended readings of this project.
No more than 100 words per answer.

Content	Progress
1. Minimal biochemistry	Done (1-minimal-biochem.docx)
1.1. variety of protein functions https://www.ncbi.nlm.nih.gov/books/NBK26911 https://chem.libretexts.org/Bookshelves/Biological_Chemistry/Supplemental_Modules_(Biological_Chemistry)/Proteins/Peptides_and_Proteins/Proteins_and_Amino_Acids	
1.2. protein structures 1.2.1. building block of protein: amino acids and their standard states https://bio.libretexts.org/Bookshelves/Biochemistry/Fundamentals_of_Biochemistry_(LibreTexts)/01%3A_Unit_I-_Structure_and_Catalysis/03%3A_Amino_Acids_Peptides_and_Proteins/3.01%3A_Amino_Acids 1.2.2. Primary, secondary and tertiary protein structures (details of 3D representations will be discussed in the next handout) *https://bio.libretexts.org/Bookshelves/Biochemistry/Fundamentals_of_Biochemistry_(LibreTexts)/01%3A_Unit_I-_Structure_and_Catalysis/03%3A_Amino_Acids_Peptides_and_Proteins/3.02%3A_The_Structure_of_Proteins-_Primary_Structure*	
1.3. Nucleic acid structures 1.3.1. Nucleotides (introduction section only) https://bio.libretexts.org/Bookshelves/Biochemistry/Fundamentals_of_Biochemistry_(LibreTexts)/01%3A_Unit_I-_Structure_and_Catalysis/08%3A_Nucleotides_and_Nucleic_Acids/8.01%3A_Nucleic_Acid_Structure 1.3.2. RNA capping (general), project specific question https://en.wikipedia.org/wiki/Five-prime_cap https://www.researchgate.net/figure/Structure-of-5-end-capped-mRNAs-The-cap-0-cap-1-and-cap-2-structures-and-5-5_fig2_293044451	

1.4. biochemical interactions 1.4.1. Types of interactions (general)	
1.5. Competitive inhibition of proteins (1st section) https://chem.libretexts.org/Bookshelves/Biological_Chemistry/Supplemental_Modules_(Biological_Chemistry)/Pharmaceuticals/Enzyme_Inhibition	
1.6. [Bonus]Minimal pharmacology and importance of selectivity 1.6.1. https://chem.libretexts.org/Bookshelves/Biological_Chemistry/Book3A_Medicines_by_Design/01%3A_ABCs_of_Pharmacology/1.02%3A_A_Drug's_Life 1.6.2. (Optional, more advanced details of the previous article) https://chem.libretexts.org/Bookshelves/Biological_Chemistry/Supplemental_Modules_(Biological_Chemistry)/Medicinal_Chemistry/Basic_Aspects_of_Drug_Activity	
2. Interpretation of 3D molecular models 2.1. 3D representations of protein structure https://bio.libretexts.org/Bookshelves/Biochemistry/Fundamentals_of_Biochemistry_(LibreTexts)/01%3A_Unit_I-_Structure_and_Catalysis/04%3A_The_Three-Dimensional_Structure_of_Proteins/4.11%3A_Biomolecular_Visualization_-_Conceptions_and_Misconceptions 2.2. Protein-ligand binding 2.2.1. https://en.wikipedia.org/wiki/Protein%E2%80%93ligand_complex 2.2.2. https://durrantlab.pitt.edu/binana/ click "use example files"	Done (2-molstruc-3D.docx)
3. Free computational chemistry resources for academic usage 3.1. Free web services 3.1.1. Uniprot https://www.uniprot.org 3.1.2. RCSB PDB https://rcsb.org 3.1.3. pubchem https://pubchem.ncbi.nlm.nih.gov/ 3.1.4. PDB2PQR server 3.1.5. (pdb quick screen/swisssimilarity/pharmit/zinc) 3.2. Software download links and installation (part 1 of demo 1) 3.2.1. Installation of computational chemistry programs 3.2.1.1. Anaconda/miniconda 3.2.1.2. Install everything in the same conda environment 3.2.1.2.1. Optional manual install	Demo0 done Handout in-progress
4. Reason of small-molecule inhibitor design 4.1. function of target protein: either journal article or uniprot 4.1.1. Search on uniprot and PDB 4.1.2. Selection of experimental structure 4.2. Why should we inhibit this protein?	Pending I may change the order of 3 and 4
5. Exercise 1: warm-up exercise and limits of quick computational model. 5.1. Fundamental of science: control test to validate your protocol 5.2. Demo1-manual-fit-eval	Work in progress: Demo and handout
6. (optional 2022) Exercise 2: application of the "standard" protocol 6.1. Workflow 6.2. Demo2-common-protocol	Work in progress: Demo and handout Scripts done

7.	(optional 2022) Exercise 3: virtual screening, another direction of structure based drug design 7.1. Workflow 7.2. Demo3-virtual-screening	All pending
8.	Optional: Molecular Dynamics	
9.	Optional: QSAR and Machine learning-based optimization	

III. Free reference materials and remarks

- Notes:
  - Libretext materials have many typos but could be ok as introductory text under creative commons license.
  - When "standard" textbook-like articles are too advanced for our purpose, more generic information from Wikipedia would be used.
- Selected chapters in
  - Selected https://chem.libretexts.org/Bookshelves/Biological_Chemistry/Supplemental_Modules_(Biological_Chemistry)/Proteins
  - Selected (still many typos) https://bio.libretexts.org/Bookshelves/Biochemistry/Fundamentals_of_Biochemistry_(LibreTexts)
  - Selected *https://www.ncbi.nlm.nih.gov/books/NBK26911*
  - https://chem.libretexts.org/Bookshelves/Biological_Chemistry/Book%3A_Biochemistry_Online_(Jakubowski)
  - https://bio.libretexts.org/Bookshelves/Biochemistry/Book%3A_Biochemistry_Free_For_All_(Ahern_Rajagopal_and_Tan)
  - (Reason: open source and mobile friendly)
- Some general information from wiki
- Uniprot data of target protein
- The RCSB PDB
- pubchem
- Swiss-target or UCSF Sea off-target prediction

IV. Further readings

- Basic PharmChem (MIT course?)
- Advanced drug design workflow recommended only for advanced final year project students who'd like to learn some programming (TeachOpenCADD, mainly jupyter notebooks written in python)
- Dated, now buggy, but still very comprehensive drug design tutorial with OPEN3DQSAR
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