**BIO215 - Bioinformatics Projects**

**(Project – II)**

1. Choose any protein sequence, run protein-protein BLAST, obtain information about the template(s), and perform modeling using MODELLER and I-TASSER. Compare the quality of your model through Ramachandran plot analysis and the SAVES server. You are free to select different software for energy minimization and side-chain refinement, such as Swiss-PdbViewer (DeepView) and SCWRL. Choose the best model and perform secondary structure analysis using PDBsum. Find active site(s) from the sequence alignment and literatures. Write your results with proper figures and references in each section.

**Examples of query sequence:**

>AIW06012.1 chitinase 2 [Thermomyces lanuginosus]

MPSFKSVVSSLPVILTALPSVQAGLDLSSTSNVVVYWGQNSAAASGGGPSQQPLATYCEDPNIDTLVMAFMTRINGAGGVPEINLANIGDSCGTFDGTNLKDCPQVGEDIKKCQSLGKTILLSIGGATYTEGGFQSAEAAEAGARMVWETFGPVTNGDALRPFGDAVVDGFDLDFEATVSNMVPFANTLRSLMDSDSSKQYFLTAAPQCPFPDAANKEMLDGAVSFDAIWVQFYNNYCGVNSYPDNFNFNTWDDWAQNTSKNKNVKVLVGVPANTGAAGSGYLPVDQLAPVIEHARTFPSFGGVMMWDASQAYANDGFLSGIKSILGSVISRVKRMFFRRDFW

>AMB61021.1 beta-xylosidase [Thermomyces lanuginosus]

MSNPKPLVTHIYTADPSAHVFNGRIYVYPSHDRETDIQFNDNGDQYDMVDYHVLSLDEPGGPVTDHGIALHMDDIPWVSKQLWAPDAAYRNGKYYLYFPARDKEGIFRIGVAVSDEPHGPFKPEPAPIPGSYSIDPAVLVDEPDASGKQKAYMYFGGIWGGQLQCWVEDPKTKQLVFDATKSGPQEPSGPGVLALGPRVAELNDDMLTFASPPREIQILDPETLQPLAADDHDRRFFEASWCHKYNGKYYFSYSTGDTHYIAYAVGDSPFGPFVYQGRILEPVVGWTTHHSIAEYKGRWWLFYHDSELSGGASHLRSVKMRELIYDENGKIHLKDPQN

>ABV69592.1 lipase [Thermomyces lanuginosus]

MRSSLVLFFLSAWTALARPVRRAVPQDLLDQFELFSQYSAAAYCAANNHAPVGSDVTCSENVCPEVDAADATFLYSFEDSGLGDVTGLLALDNTNKLIVLSFRGSRSVENWIANLAADLTEISDICSGCEGHVGFVTSWRSVADTIREQVQNAVNEHPDYRVVFTGHSLGGALATIAAAALRGNGYNIDVFSYGAPRVGNRAFAEFLTAQTGGTLYRITHTNDIVPRLPPRDWGYSHSSPEYWVTSGNDVPVTANDITVVEGIDSTDGNNQGNIPDIPSHLWYFGPISECD

2. Search for any appropriate inhibitor or ligand for your protein in the literature and perform molecular docking using AutoDock, AutoDock Vina, and Discovery Studio. For example, the inhibitor for chitinase is Allosamidin.

3. Choose the best binding pose based on binding energy and binding orientation. Generate 2D and 3D representations using Discovery Studio or PyMOL. Write your report with the following sections: Introduction, Materials and Methods, Results, Discussion, and Conclusion. You should include at least three figures and two tables in your report.