BIOINFORMATICS ASSIGNMENT 2 (Day 6 - 10)

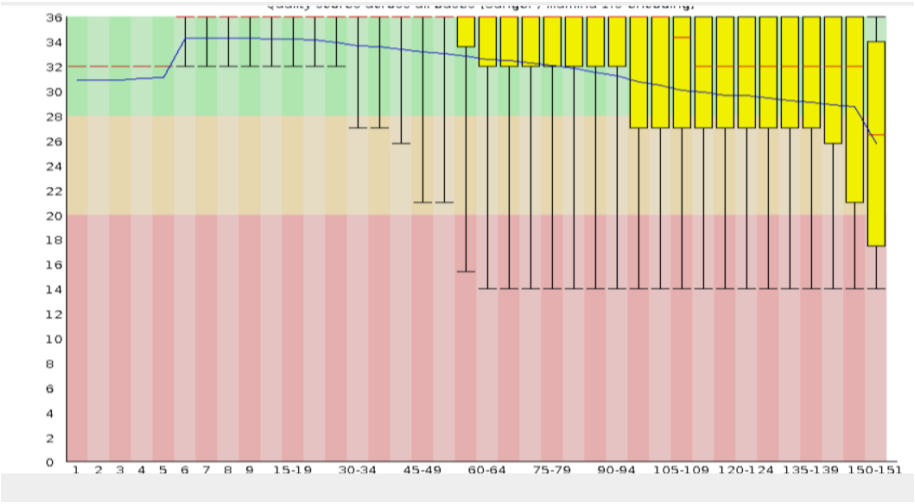
NGS DATA QUALITY CHECK (DAY 6)

1. SRA accession number: SRR24518778 [BRCA2 gene]
2. NGS platform and layout: Software name- ‘’galaxy.org’’. [Fastqc quality report]
3. Basic statistics: shows information about sequence like GC content, sequence length.

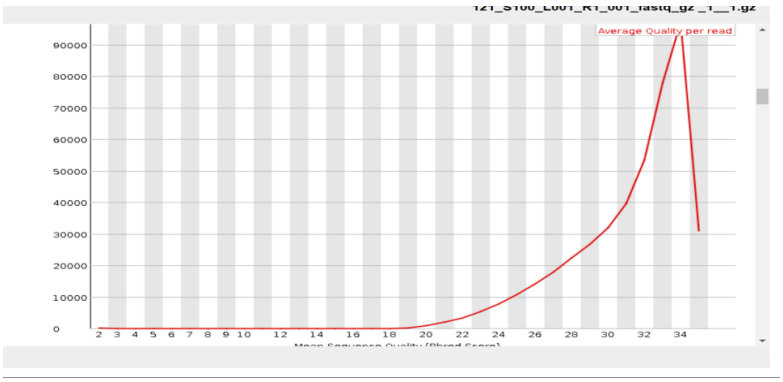
Basic Statistics

Measure	Value
Filename	121_S100_L001_R1_001_fastq_gz _1__1.gz
File type	Conventional base calls
Encoding	Sanger / Illumina 1.9
Total Sequences	444371
Sequences flagged as poor quality	0
Sequence length	35-151
%GC	38

4. Per Base sequence quality: it checks the quality of each base.the yellow box represents the interquartile range. The green region says the quality of base is good whereas the red colour shows bad quality.



5. Per sequence quality score: it checks based on phred’s code. In 1000 bases 1 error is acceptable.



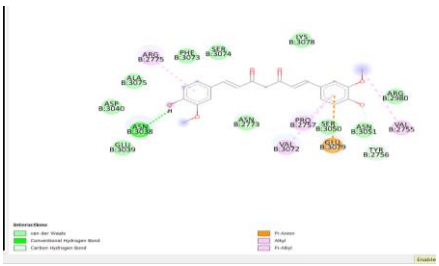
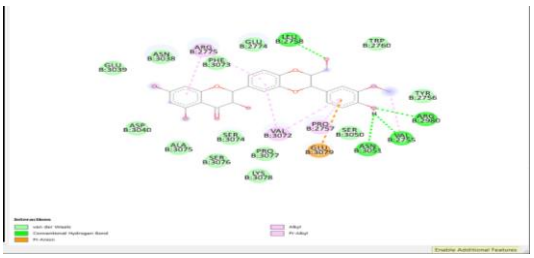
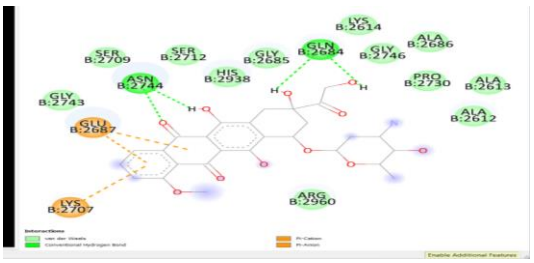
GitHub (DAY 7)

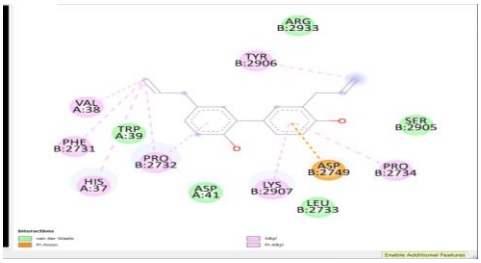
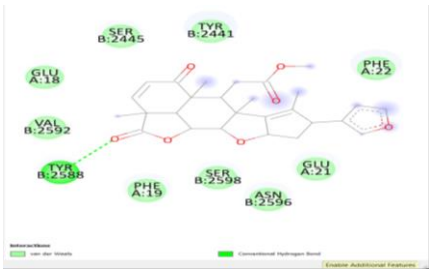
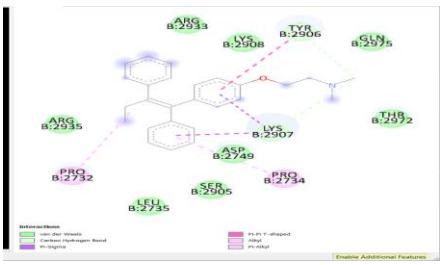
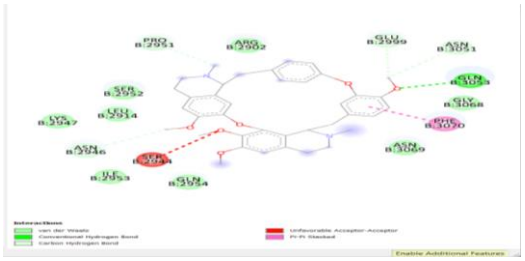
Please paste your GitHub account link - https://github.com/Neela-resh/-Summer-Internship-2023

Molecular Docking (DAY 8 and 9)

Protein Name: BRCA2 [Breast cancer type 2 susceptibility protein]

Protein ID - 1IYJ https://www.rcsb.org/structure/1IYJ

Ligand Name	Ligand ID	Energy value	Binding Affinity	Dock Image - 2D
Curcurmin	https://pubchem.ncbi.nlm.nih.gov/compound/969516	E=272.07	-7.1	
Silibinin	https://pubchem.ncbi.nlm.nih.gov/compound/31553	E=443.51	-9.1	
Doxorubicin	https://pubchem.ncbi.nlm.nih.gov/compound/31703	E=616.59	-8.1	

Honokiol	https://pubchem.ncbi.nlm.nih.gov/compound/72303#section=Structures	E=335.07	-7.3	
Nimbolide	https://pubchem.ncbi.nlm.nih.gov/compound/12313376	E=1098.41	-7.9	
Tamoxifen	https://pubchem.ncbi.nlm.nih.gov/compound/2733526	E=753.36	-6.4	
Tetrandrine	https://pubchem.ncbi.nlm.nih.gov/compound/73078	E=1026.14	-9.1	
Imidazole	https://pubchem.ncbi.nlm.nih.gov/compound/795	E=217.27	-3.4	
Lapatinib	https://pubchem.ncbi.nlm.nih.gov/compound/208908#section=Structures	E=1028.85	-7.5	

Neratinib	https://pubchem.ncbi.nlm.nih.gov/compound/9915743	E=818.89	-7.6	

RESULT: As a result, silibinin and tetrandrine drug showing highest binding affinity of 9.1Kcal whereas the compound Imidazole showing very lowest binding affinity of -3.4Kcal which is not good. The compound like imidazole, lapatinib and neratinib has no ligand is defined.

Cancer therapy: (DAY 10)

Cancer type	Hallmarks	Drug	Mechanism of drug
Breast cancer	Invasion & Metastasis	Herceptin	To block intracellular signalling pathways.
Colon cancer	Angiogenesis & stem cell characteristic of limitless replicative potential	Avastin	Avastin is designed to block a protein called VEGF. It slows down the cancer cells by lowering the blood supply to cell
Prostate cancer	Insensitivity to antigrowth signals	Alpha-blockers,such as tamsulosin(Flomax), terazosin(hytrin)	Relaxes the muscle tissue.