

Computational Technology Based Biology Project For Remote Learning During Covid-19 Crisis

S. Sheik Asraf

Department of Biotechnology,
Kalasalingam Academy of Research and Education,Krishnankoil
s.sheikasraf@klu.ac.in

Abstract: In the many months following the Coronavirus flare-up, a large number of Biotechnology Engineering students throughout the world are compelled to switch over from conventional lab based learning to computational technology based learning. This uncommon interchange enormously affected the method of learning project courses. Specifically, biological science projects which require the students and staff to work in the actual lab was affected. B. Tech. Biotechnology students and a staff from our institution utilized present day computational bioinformatics tool, data sets and programming to study an issue identified as beta-lactam resistance in a bacterium. The students utilized accessible present day computational tool, data sets and virtual products to complete the project work. This technique for doing the final year B. Tech. project has brought about the consummation of the course effectively. This procedure of utilization of freely

available computational tool, information databases and programming software will benefit the students worldwide to complete project based engineering courses effectively.

Keywords: in silico, project, workstation, COVID-19, bioinformatics

1. Introduction

Current biology based projects are utilizing traditional microbiology, biochemistry and molecular biology strategies [1, 2, 3]. Tragically, after Covid outbreak large numbers of the colleges and universities encouraging science based courses confronted the trouble in directing project based courses. In our institution, we dealt with this issue by utilizing bioinformatics tool, data sets and software. B. Tech. Biotechnology students and a staff from our institution utilized bioinformatics tool, data sets and programming software to complete the project work. NCBI- an open source database was utilized by the students for recovering the protein sequences. PROTPARAM was utilized by the students to contemplate the essential properties of protein sequences. SOPMA tool was utilized by the students for studying the secondary structural properties of the proteins. BLAST was utilized by the students to look at the grouping and characterization of protein sequences against the accessible data sets. CLUSTAL OMEGA tool was utilized by the students to examine protein groupings. SWISS-MODEL server was

S. Sheik Asraf

Department of Biotechnology,
Kalasalingam Academy of Research and Education,Krishnankoil
s.sheikasraf@klu.ac.in

utilized by the students for homology based study of protein 3D-structures. PATCHDOCK server was utilized for the docking investigations of protein with anti-microbial compound. PYMOL tool was utilized by the students to see the protein tertiary structure. CARD database was utilized for discovering the nearest relative of study proteins.

Along these lines, by utilizing such current bioinformatics tools, programming and information databases, the students were effectively able to finish the project course regardless of without admittance to wet lab tests.

2. Literature Review

The significance of proceeding with training specifically science based course during the Covid-19 pandemic has been a genuine test for both the faculty and the students [4]. Numerous colleges and universities have reimaged the new educational policies post- Covid-19 pandemic [5]. The impacts of mixed and task based learning are felt post-Covid-19 pandemic [6]. Covid-19 has opened the conduits for e-Learning based undertakings [7]. In country, for example, People's Republic of China where Coronavirus episode began, web based instruction and learning has been suggested for project courses [8]. Numerous methodologies have been made by the instructors to connect with distantly placed students after the Covid-19 episode [9]. Numerous colleges and schools have shut because of Covid related illness. This had sway upon training and psychological well-being of Undergraduate, Postgraduate and Ph.D. students and scholastic staffs that couldn't proceed with biology lab based courses [10]. Coronavirus has come as positive development and turned into motivation for instructive transformation [11]. Numerous science based instructive establishments like Schools, Colleges and Universities on the world have exchanged over to *in silico* projects [12]. In India, Coronavirus enormously affected primary, secondary, higher secondary, undergraduate, postgraduate and doctoral education [13].

3. Methodology

National Centre for Biotechnology Information genome database was utilized by the students for the recovery of protein sequences [14]. The essential primary highlights of protein sequences were found by the students by utilizing PROTPARAM tool [15].

The comparability and characteristics of the protein sequences were studied by the students using Basic Local Alignment Search Tool [16]. Different arrangement and theme investigation of protein sequences were studied by the students utilizing CLUSTAL OMEGA tool [17]. CDD was utilized by the students for looking through the moderated areas in the protein sequences [18]. The students predicted the 3D-structures of proteins by utilizing Swiss-Model server [19]. PATCHDOCK server was utilized by the students for the docking investigations of protein with penicillin. The students utilized PYMOL software to display protein tertiary structures [20]. CARD database was used for discovering the nearest of relative of proteins.

4. Result and Discussion

A. Primary structure study of proteins

The students used the Protparam tool and entered the protein sequence and the parameters of the proteins were computed. The results obtained is shown in Table. 1.

Table 1 : Predicted primary structure properties of antibiotic resistance determinant proteins and related proteins

Properties	PBPA LpoB	PBPA	AmpE	LAP-2	MreC	MreD
Number of amino acid	215	71	284	285	334	162
Theoretical pI	9.16	5.33	9.51	6.76	6.34	10.25
Stability index value	42.19	43.67	31.13	40.41	42.20	32.25
Aliphatic index value	79.86	85.67	122.22	92.39	104.16	144.94
GRAVY value	-0.268	-0.244	-0.516	-0.228	-0.047	0.998

B. Secondary structure study of proteins

The students used the SOPMA tool and entered the protein sequence and the parameters of the proteins

Table 2 : Predicted secondary structure properties of antibiotic resistance determinant proteins and related proteins

Properties	PBPA LpoB	PBPA	AmpE	LAP-2	MreC	MreD
Number of beta strands	26	69	3	17	22	7
Number of alpha helices	76	276	207	136	121	101
Others	128	374	74	132	191	54
Total residues	215	719	284	285	334	162

were computed. The number of beta strands, alpha helices and other secondary structural properties were obtained [Table. 2].

C. Basic Local Alignment Search Tool Analysis

The students used Basic Local Alignment Search Tool for protein sequence comparison. From BLASTp, the students concluded that the list of sequence producing significant alignments starts with the best match. [Table. 3].

Table. 3: BlastP analysis of antibiotic resistance determinant proteins and related proteins

Properties	PBPA LpoB	PBPA	AmpE	LAP-2	MreC	MreD
Sequences producing significant alignments	PBPA LpoB	PBPA	AmpE	ClassA Beta-lactamase	MreC	MreD
E-value	1e ⁻¹⁵³	0.0	0.0	0.0	0.0	6e ⁻¹⁰⁷

D. Motif Analysis of proteins

The students concluded that H-X-H-X-D motif, is

WP_012477595.1 IDFL-----SGKVLSHRREERFPIMSTFKVLLCGAILV
 WP_013097109.1 -----
 WP_013098986.1 -----IKP1F5RGP5LQFRLILAVLVALGVI---IA05RLGTFSQERTYMDTAVS-
 WP_020688508.1 ML-LVII---AERLFLKLG[H]DHLRLE-----VLFRR2MIFSMILRTLMLTAGVM
 WP_058679440.1 ---LQQM---S55HTRIMVQLLAIRALLKEGKTQQAAELFNLQLPHE-----LND4QRL
 WP_013098985.1 ALLLQ1MPMPDQILVYRPIMVLLILLYW-----ILALPPR-----VINGTGFL

WP_012477595.1 RVKQGLEQLERRITYKHDLDYSPLTQSQHADGHTVSELCLIAAIT[SD]VANILLSTI
 WP_013097109.1 -----
 WP_013098986.1 -----PF-----YF-IS---NGPRELLDSVSQTL---55
 WP_020688508.1 VITFLLLRSLSYGLFFVNPPLLV-----WILLGVLCLGAGKVRMHHAYHLKAASR
 WP_058679440.1 -EQSL-----S-----AEKLVALKDYAAAKKI
 WP_013098985.1 -VNGAILD-----LISGSTLGVRALSHSIAYLVAL--

WP_012477595.1 GSPE-----GLTHFLR-STGDSYTRLDRHE[S]N[AKPGDERDTTPAA
 WP_013097109.1 -----
 WP_013098986.1 RDQLELENRALRQEELLKNSELLML-GQYKQE---NARLRELLGSPRLQDEQKVNVTQ-V
 WP_020688508.1 DDA-----HARSAMASELTMIHGVP-----DCDEREFL-----
 WP_058679440.1 LGDIDVSDLKHOQARFVQAGITAEQGRPSLTLRLALIAQEPILLGGADKQKNIDATWQ-A
 WP_013098985.1 -KFLQFLRNALVQDQLWML-----SLADDIVVPMVA-E

WP_012477595.1 HAQTLQKILLNEVSLTEKSRKCLTS-----H[QEDKIVGSP]LFR-----SVLPA[HN]TAKTS
 WP_013097109.1 -----
 WP_013098986.1 IS7VMDPYSQDVW---IDK05VNGVYEQSQPVIS-DK0AVGQDQVWAV-
 WP_020688508.1 -REFLQHLLHNFHRY-----VLAFLFVUGGPVGPVLLNQVAFRLRQDTHLARY
 WP_058679440.1 LASHITQEQA-QALV7M4DMLWMLQWMLDQQWFMNARS-BPM-----MILKAGITDQTRV
 WP_013098985.1 FLVIRNSFRPPEVHCVVYQVLMPhLFLLM-----

WP_012477595.1 AGDHGSR---GIVALLGP-GKGPSPRIVV---LYITNTHSS---PHEL-----
 WP_013097109.1 -----
 WP_013098986.1 -----AKLTSRVLILLICDATHALPTQVLRVNDERIAAGNGCTD0BQLEHLPAINTDQVGD
 WP_020688508.1 LTPLHE-RLLSGIDAIYLHDLMLPYRLVSVVY-AI0HSEKA-----LP-----
 WP_058679440.1 PQ[IPGAKN]LP---TQLMVNQIFK[PAST]KIAL--LLPUNQVA-----
 WP_013098985.1 -----

WP_012477595.1 EHIA6IGD5V1W-----[K]KHSISRYAL-----TAFAFLPL4QCVT-----
 WP_013097109.1 -----
 WP_013098986.1 LVT56LQ6RPFEDYQPVWAVVSSV[KL]DTQHAYTTV1QDPTA6QDQRLKYLLELHQDQHKA[P]
 WP_020688508.1 AH[AS]LGDQRTSQVQL-----
 WP_058679440.1 ---VFGRT1DQGFEM-----[K]C[TP]
 WP_013098985.1 -----RIVRQQFAWQ-----

WP_012477595.1 -----RTEQPA[PVDE]L[K]P[QPTQ]P[D]P[D]P-----
 WP_013097109.1 -----
 WP_013098986.1 MTPPEEVHRY-----AHLRLQNPQVW-[P]PQV-[S]PP-----APU-----[S]
 WP_020688508.1 -----R[Q]QFSLAREPHDQK1ETP-----KARVSM-----AKK
 WP_058679440.1 VTE5AVPAGAQQQAAQAMIDVWSPSAETSLDTAQTQPPQGTHQIP-----VTA[PT]PRAAAMPA
 WP_013098985.1 -----

Fig.1: Motif analysis of the beta lactam resistant protein

present in Multispecies: beta-lactamase regulatory AmpE(wp_020688508.1) and S-X-N motif is present in Multispecies: penicillin binding protein activator and Multispecies :class A beta-lactamase LAP-2(wp_058679440.1 and wp_012477595.1). Students found that S-V-V motif is present in Multispecies: Rod shape determining protein mreD (wp_013098985.1) K-X-G motif is present in Multispecies:

penicillin binding protein activator LpoB and Multispecies: penicillin binding protein activator and Multispecies: Class A beta lactamase LAP-2(WP_012477595.1 and wp_013097109.1) was found out by the students [Fig. 1].

E. Homology Modelling and docking analysis

The homology modeling of the proteins performed by the students gave the fundamental underlying highlights of the proteins namely the alpha helix, beta structure and a functioning serine amino acid residue



Fig. 2 : Protein docked with antibiotic

known for annihilating the beta lactam ring of penicillin. The cooperating side chains are shown as ball and stick. The arrangement and layout structure are then utilized by the students to deliver underlying model of the objective. The precision of the designs produced by the students is exceptionally subject to the succession character among target protein and database template protein [Fig. 2].

F. Docking Analysis of proteins

PatchDock utilizes a math based docking programming. The students uploaded the structures of protein and penicillin as input. The yield acquired by the students showed a rundown of potential protein-penicillin docked structures.

The Receptor and Ligand in Protein Data Bank design was transferred by the students. The Protein Data Bank design was recovered from the Swiss-model server and the antibiotic Protein Data Bank

structure was recovered utilizing Pubchem. The PDB design atoms in the antibiotic and protein were prepared. A home address that addresses the main 20 arrangements of docked protein-penicillin complex was created. The statistical value, the size of the interaction and the change of the arrangement were acquired. The Protein Data Bank document of the protein-penicillin complex was recovered as a packed record that contains the high scored values [Fig.3].

In this way, by utilizing such present day computational tools, programming and information databases, the students were effectively able to finish the project course work notwithstanding without admittance to wet lab tests.

4. Conclusion

After Coronavirus lockdown, numerous colleges, universities and schools have introduced innovation in teaching and learning process [21]. Essentially, our

PATCHDOCK + ?

Molecular Docking Algorithm Based on Shape Complementarity Principles

[\[About PatchDock\]](#) [\[Web Server\]](#) [\[Download\]](#) [\[Help\]](#) [\[FAQ\]](#) [\[References\]](#)

Receptor	Ligand	Complex Type	Clustering	RMSD	User e-mail	Receptor Site	Ligand Site	Distance Constraints
model.pdb	tclactv0009sBvDy.pdb	Default	4.0	9917001057@klu.ac.in	-	-	-	-
<hr/>								
Solution No	Score	Area	ACE	Transformation	PDB file of the complex			
1	4430	572.10	-77.87	2.15 -0.50 1.60 2.05 1.52 34 196.67	result.1.pdb			
2	4372	539.50	-90.04	0.32 0.88 -1.71 1.52 1.52 50 196.52	result.2.pdb			
3	4316	575.20	-141.51	-1.92 0.53 1.61 1.82 1.51 58 201.40	result.3.pdb			
4	4120	543.70	-241.92	-2.63 0.98 -0.37 0.31 155.90 190.42	result.4.pdb			
5	4100	479.80	-78.82	2.13 0.57 -2.73 -1.17 147.02 200.57	result.5.pdb			
6	4060	557.10	-152.45	0.92 -1.15 2.60 1.23 155.67 192.09	result.6.pdb			
7	4034	498.50	-160.31	-1.00 0.08 0.24 0.51 146.59 198.77	result.7.pdb			
8	3990	514.30	-144.88	2.83 1.32 -2.82 1.90 155.35 198.97	result.8.pdb			
9	3976	442.20	-126.36	0.51 0.77 1.53 2.36 157.82 196.93	result.9.pdb			
10	3938	506.50	-154.90	-1.04 -0.37 2.33 29.14 144.94 180.83	result.10.pdb			
11	3926	544.00	-163.10	-0.68 -0.89 -1.18 0.75 150.64 202.23	result.11.pdb			
12	3920	479.30	-115.53	-1.84 0.31 -0.91 29.45 145.60 180.85	result.12.pdb			
13	3878	526.20	-192.23	0.68 -0.35 -2.98 -3.39 147.83 196.07	result.13.pdb			
14	3872	463.50	-44.76	0.42 -0.53 1.50 -0.85 149.98 196.58	result.14.pdb			
15	3862	414.60	-188.38	1.36 -0.54 0.14 14.80 157.75 183.17	result.15.pdb			
16	3848	517.10	-124.47	-0.28 1.07 2.28 0.57 149.91 202.69	result.16.pdb			
17	3846	434.20	-69.29	1.68 -0.22 -3.02 -1.34 155.21 193.55	result.17.pdb			
18	3812	422.20	-190.44	-0.85 -1.04 -1.25 30.55 153.47 193.55	result.18.pdb			
19	3800	426.30	-83.88	-2.66 -0.45 0.33 -2.05 147.07 201.22	result.19.pdb			
20	3794	520.20	-115.96	-2.81 0.66 -1.56 -0.05 150.54 195.55	result.20.pdb			

Fig.3 : Beta-lactamase (WP_0130998985.1 MULTISPECIES: rod-shape determining protein MreD) docked with antibiotic

B. Tech. Biotechnology students likewise have used bioinformatics based tools, software and programs for finishing the project. There are numerous science based project courses have adjusted to innovation based U.G. research projects during the Coronavirus lockdown [22].

Our students used the cutting edge computational tools, data sets and programming software to do the project work. List of schooling, for example, colleges and universities during the lockdown time of Coronavirus pandemic has become normal [23]. Data innovation has been utilized by a capstone project during lockdown [24]. Since, the outbreak of Coronavirus, we likewise utilized present day *in silico* tools for this capstone project [25].

Numerous educational institutions have been using online science learning as done by us with assistance of computational tool, software and database [26]. This technique for utilizing the cutting edge bioinformatics tool, data sets and programming software worldwide to completed project based courses effectively. This procedure of utilization of openly accessible freeware will help students. Besides, a perplexing research objective of antibiotic resistance was studied by us without spending any reagents and other wet lab prerequisites.

Consequently, we recommend the use of computational tools for complex exploration undertakings, for example, mini projects, experientially learning projects, minor and major projects offered by the educational institutions everywhere on the world. However, we accept that traditional wet lab analyses will additionally improve our insight about the investigation like antibiotic resistance in microscopic organisms.

Online project classes can be conducted safely by following the guidelines: 1. Closing the social media sites and applications, 2. Limiting the smartphone usage and doing the experiments only in computer, 3. Turning off the phone and leaving it in out of reach, 4. Creating a schedule in social media.

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