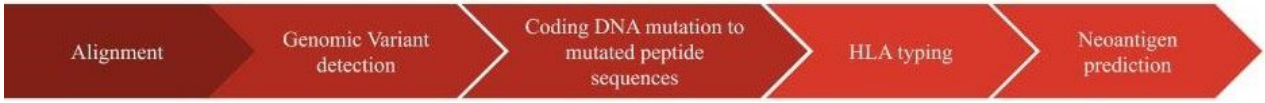
Existence of endemic viruses and their likely zoonotic transmission bells an alarm for development of population specific vaccines. Computational prediction of neoantigens not only serves the purpose of vaccine design against viruses but also for personalised immunogenic therapy.

Entire study is performed over public GALAXY server - GALAXY Europe - https://usegalaxy.eu/. Schematic execution of the workflow is as follows.



We can incorporate and try various options of available aligners and variant callers like BWA-MEM, Bowtie2, STAR, HISAT2, GATK, VARSCAN, FreeBayes etc. while forming GALAXY workflows.

Genomic variant detection (results are combined together)	https://usegalaxy.eu/u/ambarishk/w/gatk4
	https://usegalaxy.eu/u/ambarishk/w/varscan
HLA typing and neoantigen prediction	https://usegalaxy.eu/u/ambarishk/w/neo-antigen-prediction

Table-01: Shared and published GALAXY workflows incorporated into the present study.

Preliminary result is based upon SARS-CoV-2 infected human RNASEQ paired-end illumina reads obtained from SARS-CoV-2 infected Wuhan, China population. SRR accession - SRR11454612. Tabulated results are top ranked neoantigens generated from mitochondrially encoded cytochrome c oxidase I.

allele	length	peptide	ic50	percentile_rank
HLA-A*24:02	9	TYAKIHFTI	6.6	0.02
HLA-A*24:02	9	LYQHLFWFF	14.4	0.03

Table-02: Predicted MHC class I neoantigen using netmhcpan method.

allele	length	peptide	ic50	rank
HLA-DRB1*15:01	12	YILILPGFGMIS	67.19	0.1
HLA-DRB1*15:01	12	VYILILPGFGMI	67.33	0.1

Table-03: Predicted MHC class II neoantigens using netmhcpan method.

allele	length	peptide	proteasome_score	tap_score	mhc_score	processing_score	total_score	ic50_score
HLA-A*24:02	9	LYQHLFWFF	1.466175	1.2064229672	-1.31597034546	2.6725979672	1.35662762174	20.7
HLA-A*24:02	9	MFIGVNLTF	1.432985	1.2271636708	-1.44870631991	2.6601486708	1.21144235089	28.1

Table-04: Predicted MHC I processing using netmhcpan method

Position	Residue	Start	End	Peptide	Score
3	A	1	5	MFADR	0.854
4	D	2	6	FADRW	0.926

Table-05: Antibody epitope prediction using Chau-Fasman method

Shared GALAXY history - https://usegalaxy.eu/u/ambarishk/h/neo-antigen-prediction

Extended work will include development of a workbench as a dedicated GALAXY server for neoantigen prediction and antigenicity analysis as well as generation of results for all virus infections whose vaccines are under development and diseases requiring personalised neoantigen therapy. It will be an effective computational platform for population specific and personalised neoantigen therapy. As a collaborative and shared effort we will be working along with Galaxy for proteomics (Galaxy-P) team at the University of Minnesota, USA. Associated aspects with computational prediction of neoantigens over GALAXY are automation, reproducibility, time and cost-effectiveness.

References

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