

Homology Modeling Epitopes of Kirsten Rat Sarcoma (KRAS) G12D, G12V and G12R as Pancreatic Ductal Adenocarcinoma Vaccine Candidates

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Details



Primary Language: English

**Abstract (en)**

Pancreatic ductal adenocarcinoma (PDAC) is among the world's deadliest cancers. Multiple studies demonstrated that PDAC is frequently characterized by the presence of Kirsten Rat Sarcoma (KRAS) G12D, G12V, and G12R protein mutants. The mutants are potential immunotherapy targets due to their potential as cancer-specific neoantigens. KRAS G12D, G12V and G12R contain vaccine-immunogenic epitopes. KRAS G12D, G12V and G12R epitopes were presented at major histocompatibility complexes (MHC) class I. The rational design of peptide vaccines to enhance the efficacy of cancer immunotherapy is facilitated by developing a peptide structural data library and knowledge of the MHC and antigen presentation processes. Before predicting peptide activity against MHC, homology modeling must transform the peptide into a three-dimensional structure. In this study, I-TASSER was used to perform homology modeling with the assistance of other applications. In silico methods for predicting epitopes to produce

rationally designed peptide vaccines can increase the efficacy of these vaccines. This study yielded four epitope models that are potential PDAC vaccination candidates, KSFEDIHHYR, GIPFIETSAK, VVVGARGVGK and VVVGADGVGK.

### Keywords (en)

Homology Modeling, Epitope, KRAS, Vaccine, PDAC

### References

1. <https://gco.iarc.fr/today/home>, 2020, Accessed: 29.06.2022.
2. J. Earl, S. Garcia-Nieto, J.C. Martinez-Avila, J. Montans, A. Sanjuanbenito, M. Rodríguez-Garrote, E. Lisa, E. Mendiá, E. Lobo, N. Malats, A. Carrato, C. Guillen-Ponce, Circulating tumor cells (Ctc) and kras mutant circulating free Dna (cfdna) detection in peripheral blood as biomarkers in patients diagnosed with exocrine pancreatic cancer, BMC Cancer 15 (1) (2015) 1–10.
3. <https://www.cancervic.org.au/research/vcr/cancer-fact-sheets/pancreatic-cancer.html>, May 2022, Accessed: 29.06.2022.

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### Additional Information



#### Supporting Institution

Research and Development Institute of Universitas Muhammadiyah Prof. DR. HAMKA

#### Project Number

174 / F.02.09 / 2019

#### Thanks

Special thanks for the assistance



There are no additional information.

Journal Full Title: *Turkish Computational and Theoretical Chemistry*

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Decision Letter



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### Decision Letter-1

Dear Yeni YENİ,

**Decision:** Accepted

**Decision Date:** September 9, 2022

#### Reviewer Reviews

##### Reviewer-1

1. Comment For Editor:

*-It was a pleasure to review this article of importance in its field. I found the research question was clearly stated and well expressed objectives. The methods applied were seems to be appropriate and fully described in the article. Similarly, the results section well furnished, illustrative and self-explanatory enough, to answer the questions posed at the beginning. Considering the applicability and utility of the work, I recommend the acceptance of the paper in its present form.*

**Comments and Suggestions for Author:** It was a pleasure to review this article of importance in its field. I found the research question was clearly stated and well expressed objectives. The methods applied were seems to be appropriate and fully described in the article. Similarly, the results section well furnished, illustrative and self-explanatory enough, to answer the questions posed at the beginning. Considering the applicability and utility of the work, I recommend the acceptance of the paper in its present form.

**Recommendation:** Accepted

##### Reviewer-2

1. Comment For Editor:

*-In my opinion, this manuscript deserves to be published in Turkish Computational and Theoretical Chemistry .*

**Comments and Suggestions for Author:** In my opinion, this manuscript deserves to be published in Turkish Computational and Theoretical Chemistry .

**Recommendation:** Accepted

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