

Rational Development of a Therapeutic Peptide Vaccine Targeting Tumor-Specific Antigens in Neuroblastoma

What is Neuroblastoma?



Neuroblastoma is a type of cancer that effects immature nerve cells (neuroblasts).

This means it targets infants and children

Around 5500 cases of neuroblastoma are recorded every year globally affecting thousands of children.



Cancer Vaccine

IL-2, IFN γ , TNF

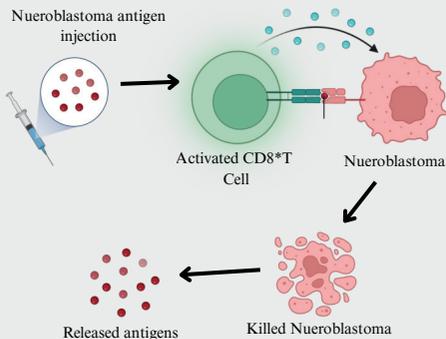


Figure 1: Shows us a vaccine that can help activate B Cell and help kill the Neuroblastoma cell. The image was made by student using biorender and canva.

Hypothesis

I hypothesize that epitope E1 (Tumor-specific antigens) binds strongly to the B-cell receptors (CD79a and CD79b) and can be used to develop a peptide vaccine against neuroblastoma.

Objectives

To identify tumor-specific antigens using computational simulations for the design of a peptide-based cancer vaccine targeting neuroblastoma.

Methodology

Epitope

The Neuroblastoma epitopes were obtained from the Immune Epitope Database & Tools



AlphaFold3

I used it to find the shape of a B-cell receptor (BCR) which makes it easier to analyze.



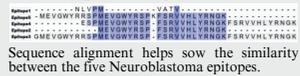
P2Rank

I used it to help find the binding site of the B-cell receptor and further helped to visualize the protein.



Sequence Alignment

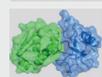
Sequence alignment helps show the similarity between the five Neuroblastoma epitopes.



Protter & The Human Protein Atlas

Protter showed where and how the individual amino acids in the BCR were organized. The Human Protein Atlas was used to find the Neuroblastoma epitopes.

GRAMM



GRAMM

Molecular Docking Simulation: This helped me use protein docking to find where the Neuroblastoma epitopes would bind with the BCR.

CD79-Epitope interaction: PLIP

Molecular docking analysis helped to provide more information concerning how the BCR and the epitopes would bind, such as the hydrophobic interactions and hydrogen bonds.

Results

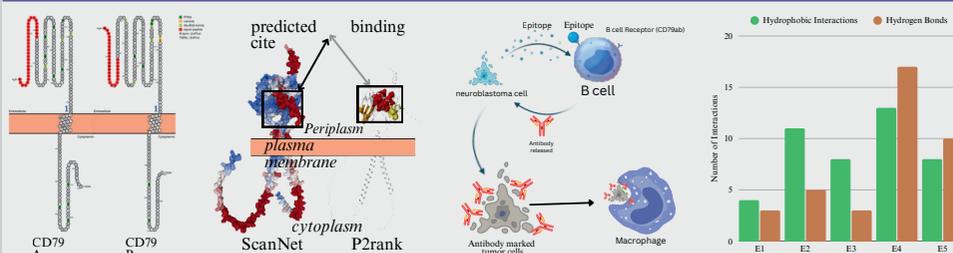


Figure 2: Shows us model of the B cell receptor. The image was made using Protter.

Figure 3: Shows us B Cell receptor and where the antigen binds. The image was made using ScanNet (deep learning) and P2rank (machine learning).

Figure 4: Shows how B Cell uses different chemical bonding's to destroy the neuroblastoma cell. The image was made using Canva and Prodigy.

Figure 5: Shows us a graph of different chemical bonding's between BCR and epitopes. The image was made using Plip Websverer.

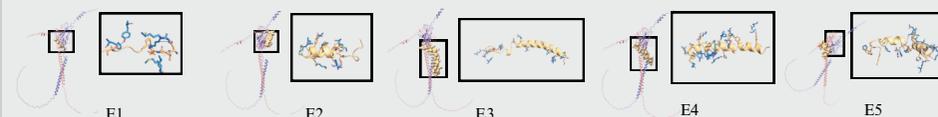


Figure 6: Shows us different epitopes (parts of antigen) of the Neuroblastoma cell and where it binds on the B-Cell receptor. The image was made by student using Chimera X.

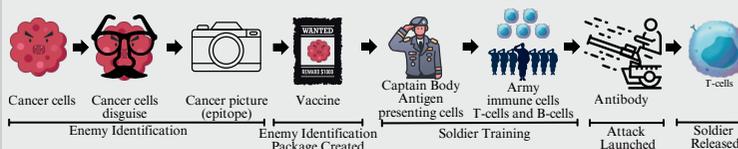


Figure 7: Shows us the process on how cancer cells are found and attacked on. The image was made using Canva.

Discussion

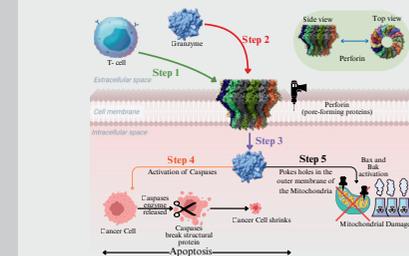


Image 8: shows how the killer t cell releases granzyme's and perforin which kill the cancer cells; Made by using biorender

Conclusion

- CD79a and CD79b were identified as tumor-specific targets for neuroblastoma.
- AlphaFold 3 and P2Rank accurately modeled receptor structures and binding sites.
- Docking and PLIP analysis confirmed strong epitope (E4) interaction and the hypothesis was rejected.
- In silico methods show promise for peptide vaccine design in neuroblastoma.

APPLICATION

- This pipeline can be used to screen and identify vaccine targets against other pediatric cancers.
- The antigenic regions identified may serve as leads for peptide vaccine development and further immunogenicity testing.

FUTURE WORK

- Test the predicted peptides in wet-lab immunoassays to confirm their antigenicity and immune response potential.
- Expand the pipeline to analyze more neuroblastoma-specific antigens and simulate T-cell epitope responses.

References

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