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Structural Analysis of Saxitoxin and Neosaxitoxin Toxins with Potential Therapeutic Targets

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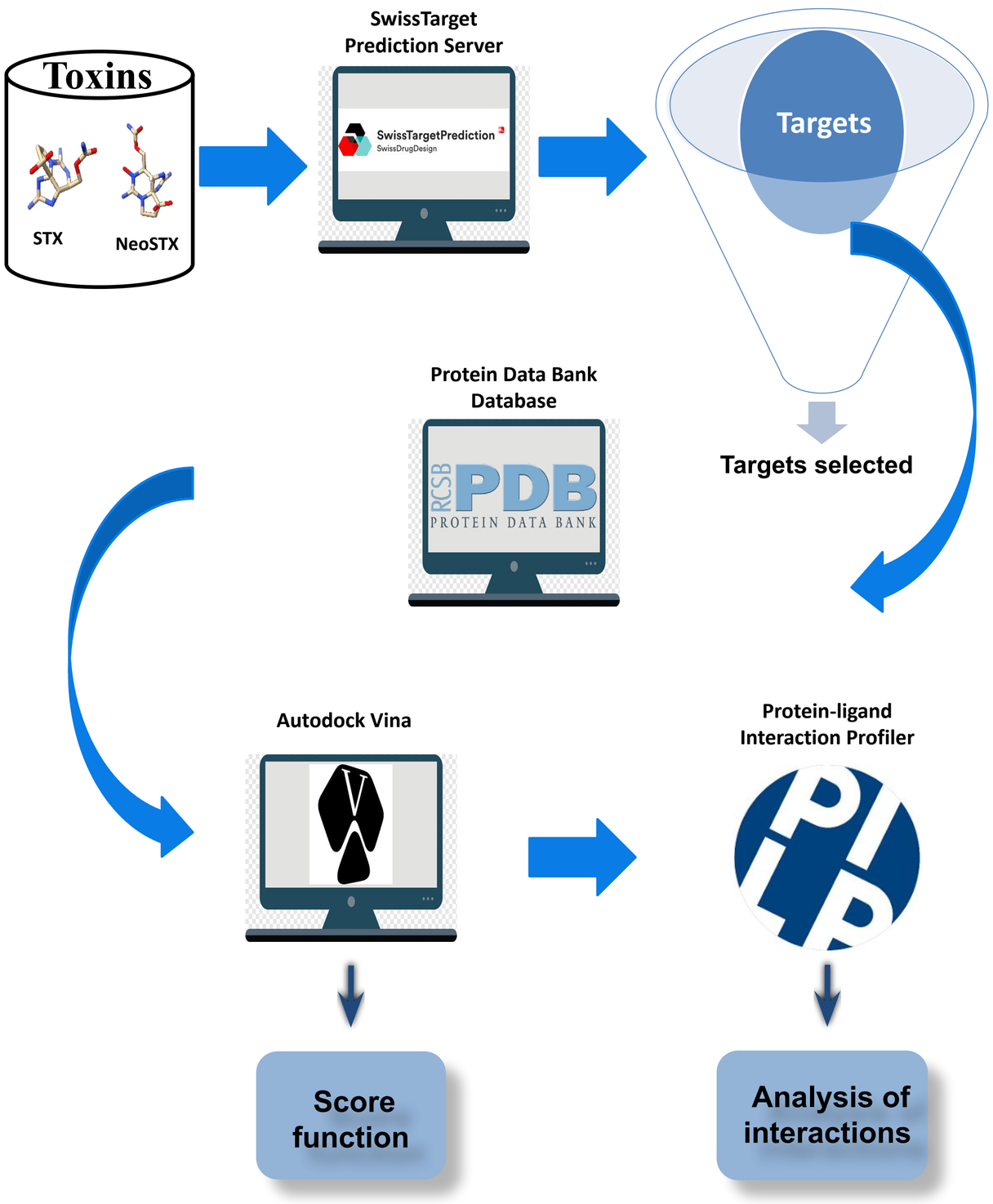
INTRODUCTION & AIM

Throughout History, there have been several events of toxins being used as biological weapons, including marine toxins produced by dinoflagellates, diatoms, bivalve mollusks and other filter-feeding organisms, such as cyanobacteria. Furthermore, they may be associated with food seafood poisoning. Despite being potentially toxic, the marine toxins present a vast chemical and biological diversity, making them an exceptional reservoir for discovering new medicines. Saxitoxin (STX) is a powerful paralyzing marine toxin from dinoflagellates and cyanobacterias. Aiming at the value of exploring marine toxins and other associated bioactive molecules as a source of potential therapeutic agents for biotechnological applications. In this work, we investigated STX and NeoSTX abilities bind to targets using *in silico* methodologies.

The objective of this study is to evaluate the binding mode of STX to different targets, study its dynamic behavior and the in vitro consequences of their interaction and propose paths of therapeutic activities for STX.

METHODS



RESULTS & DISCUSSION

Table 1. Results of SwissTargetPrediction server.

SwissTargetPrediction server	
STX	**NeoSTX**
Serotonin 6 (5-HT6) receptor **Carbonic anhydrase XII** **Tyrosinase** **C-X-C chemokine receptor type 3** **Steryl-sulfatase** **Nuclear receptor subfamily 4 group A member 1** **Carbonic anhydrase II** **Carbonic anhydrase I** **Carbonic anhydrase IX**	

Table 2. Results of AutoDock Vina program from HTR6 receptor with toxins.

AutoDock Vina program	
Toxins	**Score**
STX	-5.5
NeoSTX	-5.7

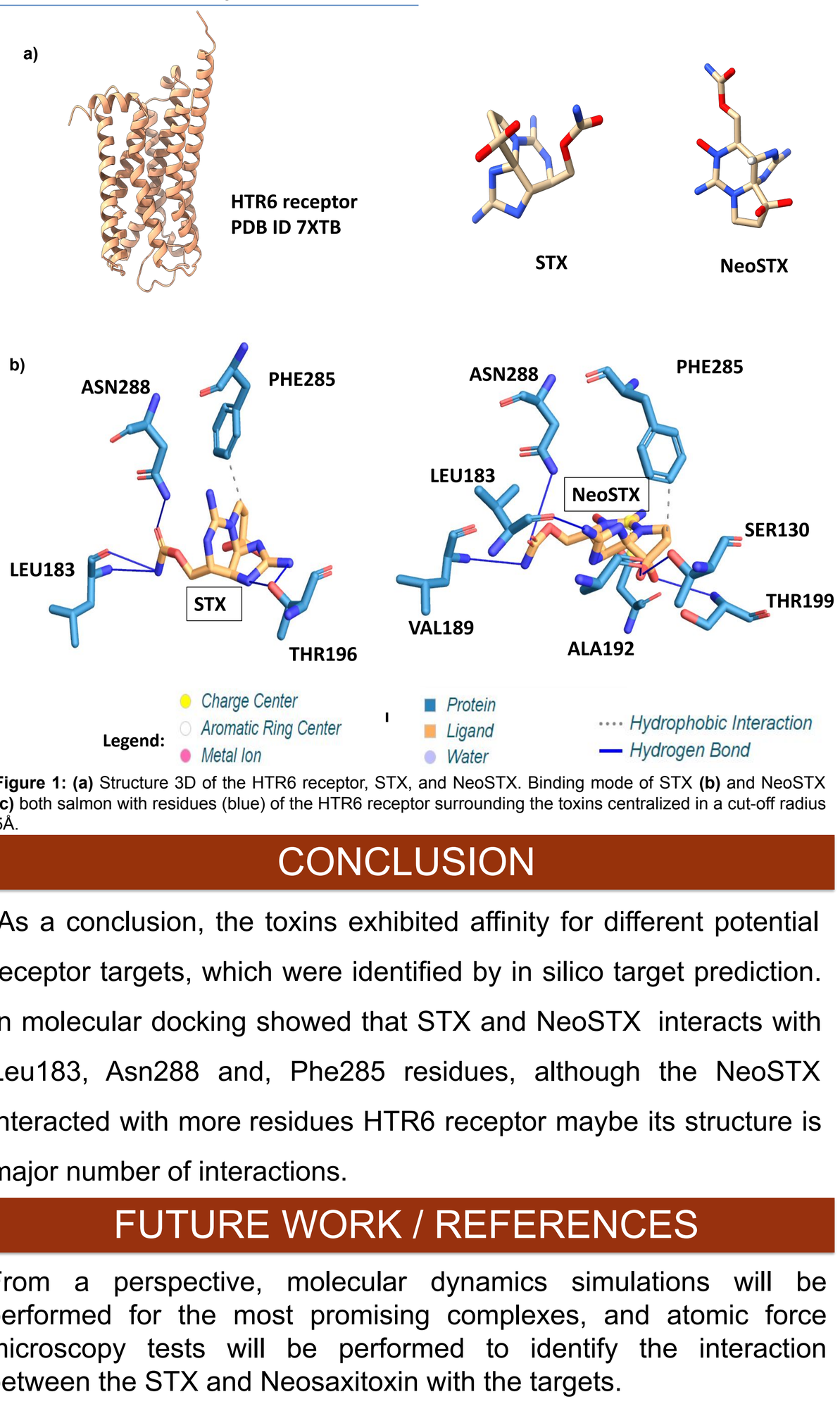


Figure 1: (a) Structure 3D of the HTR6 receptor, STX, and NeoSTX. Binding mode of STX **(b)** and NeoSTX **(c)** both salmon with residues (blue) of the HTR6 receptor surrounding the toxins centralized in a cut-off radius 5Å.

CONCLUSION

As a conclusion, the toxins exhibited affinity for different potential receptor targets, which were identified by in silico target prediction. In molecular docking showed that STX and NeoSTX interacts with Leu183, Asn288 and, Phe285 residues, although the NeoSTX interacted with more residues HTR6 receptor maybe its structure is major number of interactions.

FUTURE WORK / REFERENCES

From a perspective, molecular dynamics simulations will be performed for the most promising complexes, and atomic force microscopy tests will be performed to identify the interaction between the STX and Neosaxitoxin with the targets.