IOCT 2025 Conference
The 3rd International Online Conference on Toxins
10–12 September 2025 | Online
MDPI

Structural Analysis of Saxitoxin and its analogs: a Computational Study

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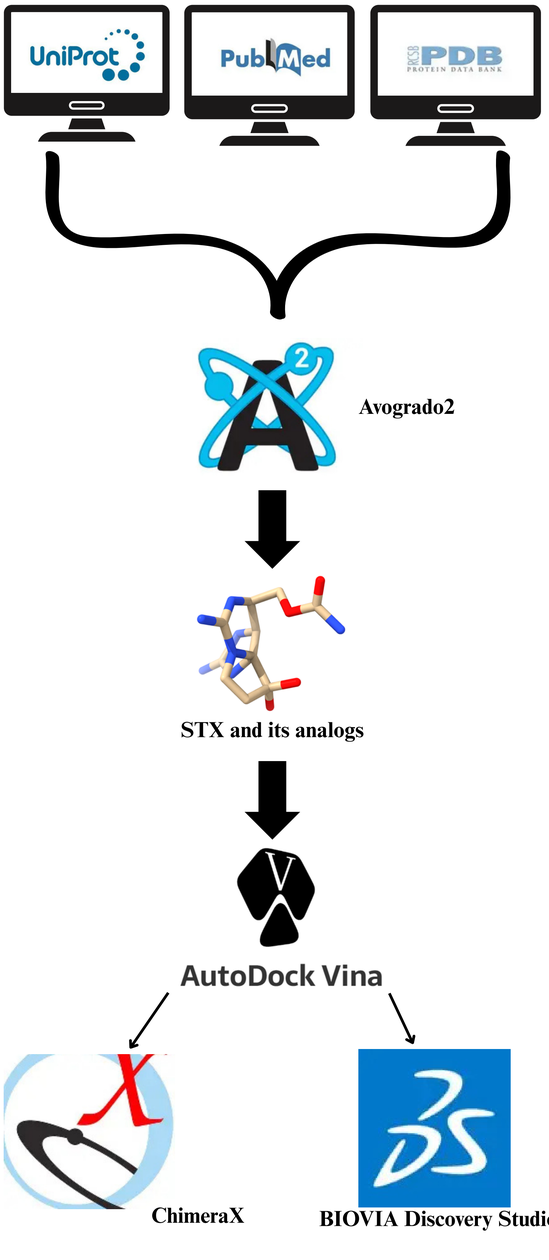
INTRODUCTION & AIM

The three-dimensional structure of saxitoxin reveals a complex, highly symmetrical molecule featuring a polycyclic, fused ring system. Saxitoxin is a potent neurotoxin primarily associated with paralytic shellfish poisoning (PSP). When ingested, it can cause a range of symptoms, including tingling or numbness around the lips, face, and neck. As the toxin's effects progress, it can lead to more severe symptoms such as muscle weakness, difficulty breathing, and in extreme cases, paralysis. Ingesting high levels of saxitoxin can be life-threatening, as it can cause respiratory failure due to paralysis of the respiratory muscles. It is crucial for individuals to avoid consuming contaminated shellfish to prevent poisoning. This project focuses on saxitoxin and its analogs, including GTX5, GTX2, and C1. It explores their chemical structures, toxicological properties, and interactions with biological systems, aiming to understand their mechanisms and potential impacts.

Understanding the structure of saxitoxin is essential for developing detection methods and potential antidotes, as well as for understanding its mechanism of action at the molecular level.

METHODS

In silico studies refer to research conducted through computer simulations and computational models, rather than traditional laboratory experiments. For this work, a computational *in silico* study was performed on saxitoxin and its analogs GTX5, GTX2, and C1. Below, we have a diagram that provides a detailed illustration of how this *in silico* study was conducted.



RESULTS & DISCUSSION

Table 1. Results of Autodock Vina program from Saxiphilin with ligands.

LIGANDS	SCORE
Saxitoxina (STX)	-8,1 Kcal/mol
GTX5	-7,8 Kcal/mol
GTX2/3	-9,2 Kcal/mol
C1/2	-7,5 Kcal/mol

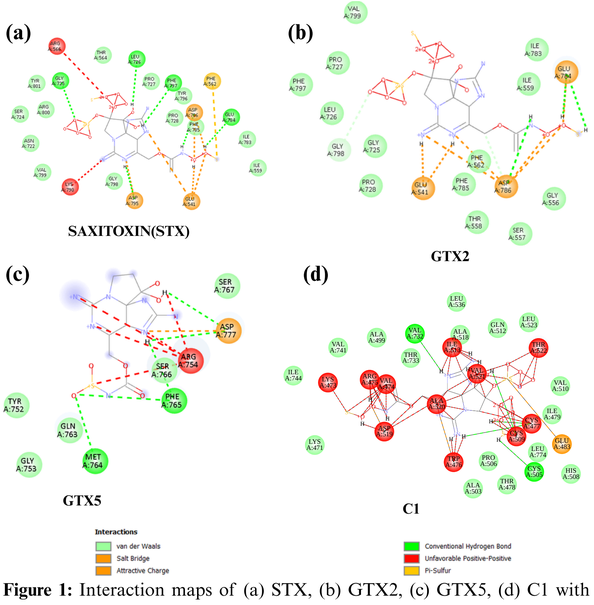


Figure 1: Interaction maps of (a) STX, (b) GTX2, (c) GTX5, (d) C1 with residues of Saxiphilin receptor surrounding the ligands centralized in a cut-off radius 5Å.

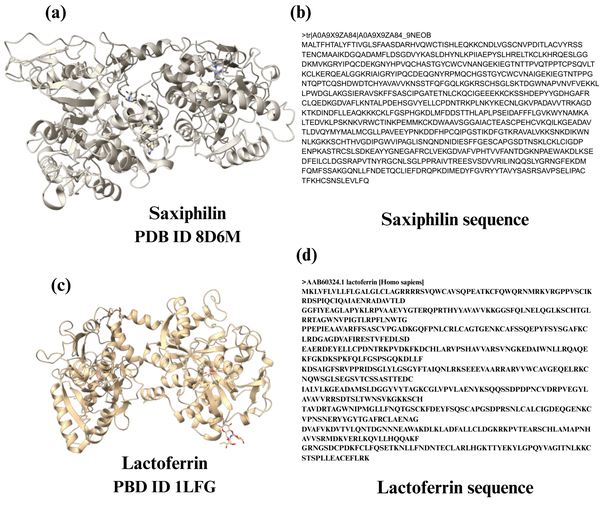


Figure 2: (a) Structure 3D and (b) sequence of the Saxiphilin, (c) Structure 3D and (d) sequence of the Lactoferrin.

CONCLUSION

In summary, it was observed that the common molecules and residues present in all complexes — STX, GTX5, GTX2, and C1 — are: Aspartate (Asp), Glutamate (Glu), Arginine (Arg), Lysine (Lys), and some polar residues such as Threonine (Thr), Serine (Ser), Glutamic acid (Glu), and Asparagine (Asn). These findings allowed the identification of common interactions, including hydrogen bonds between the guanidinium group of the toxin and acidic residues (Asp/Glu), electrostatic interactions (positive charge of the toxin interacting with the negative charge of the residues), and contacts with polar residues located near the binding site (Ser, Thr, Asn, Gln).

FUTURE WORK / REFERENCES

As a perspective, we hope to be able to carry out new docking simulations using Lactoferrin with ligands.