

Leveraging Data-Driven AI to Explore Plant-Based Compounds for Neuroinflammation and Inflammatory
Receptor Modulation via Polypharmacology

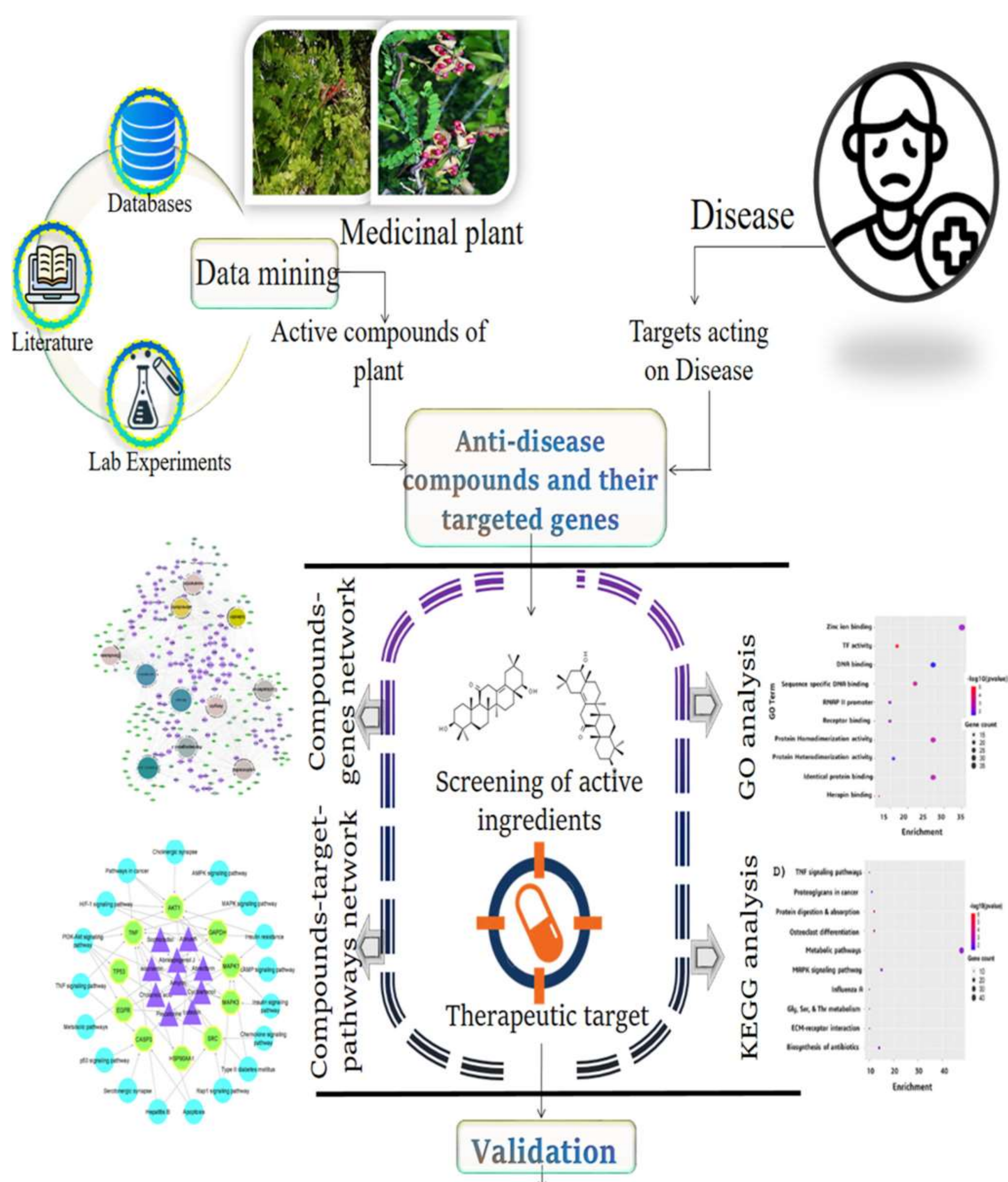
Presented by

Ranajit Nath¹, Rajesh E Jesudasan^{1*}¹School of Pharmacy, The Assam Kaziranga University, Jorhat 785006.

INTRODUCTION & AIM

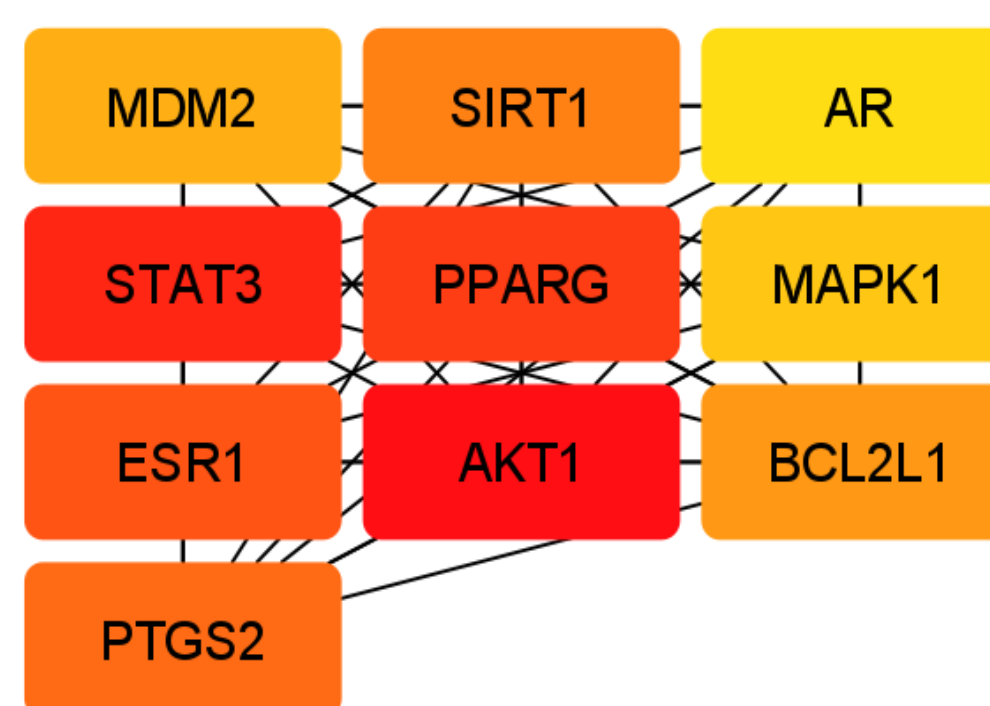
- ✓ □ Natural compounds have played a pivotal role in the realm of medicine due to their capacity to interact with and affect cellular targets involved in various diseases.
- ✓ □ Network pharmacology has emerged as an intriguing and systematic approach within this domain, enabling a comprehensive exploration of traditional medicines and their intricate bio-active constituents.
- ✓ □ Inflammation and pain are complex physiological responses that can become long-lasting health issues. They involve an intricate network of molecules and receptors, making their clinical management challenging.
- ✓ □ *Cyamopsis tetragonoloba* is renowned for its strong antioxidant properties and is well-regarded for its numerous health benefits. These advantages encompass its potential to potentially aid in preventing prostate enlargement, reducing bladder and urethral pressure while improving bladder function, supporting diabetes management by lowering blood sugar levels, and potentially lowering the risk of gastric, breast, lung, and colorectal cancers. *Cyamopsis tetragonoloba* are cultivated in various regions throughout India and in warm climates around the world.

METHOD

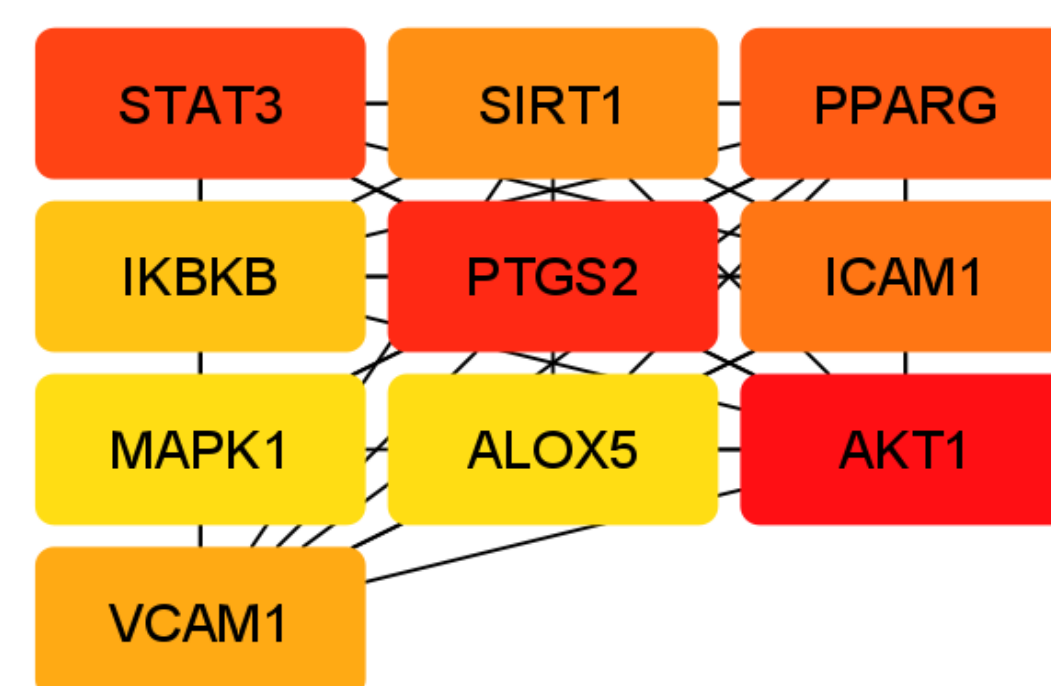


RESULTS & DISCUSSION

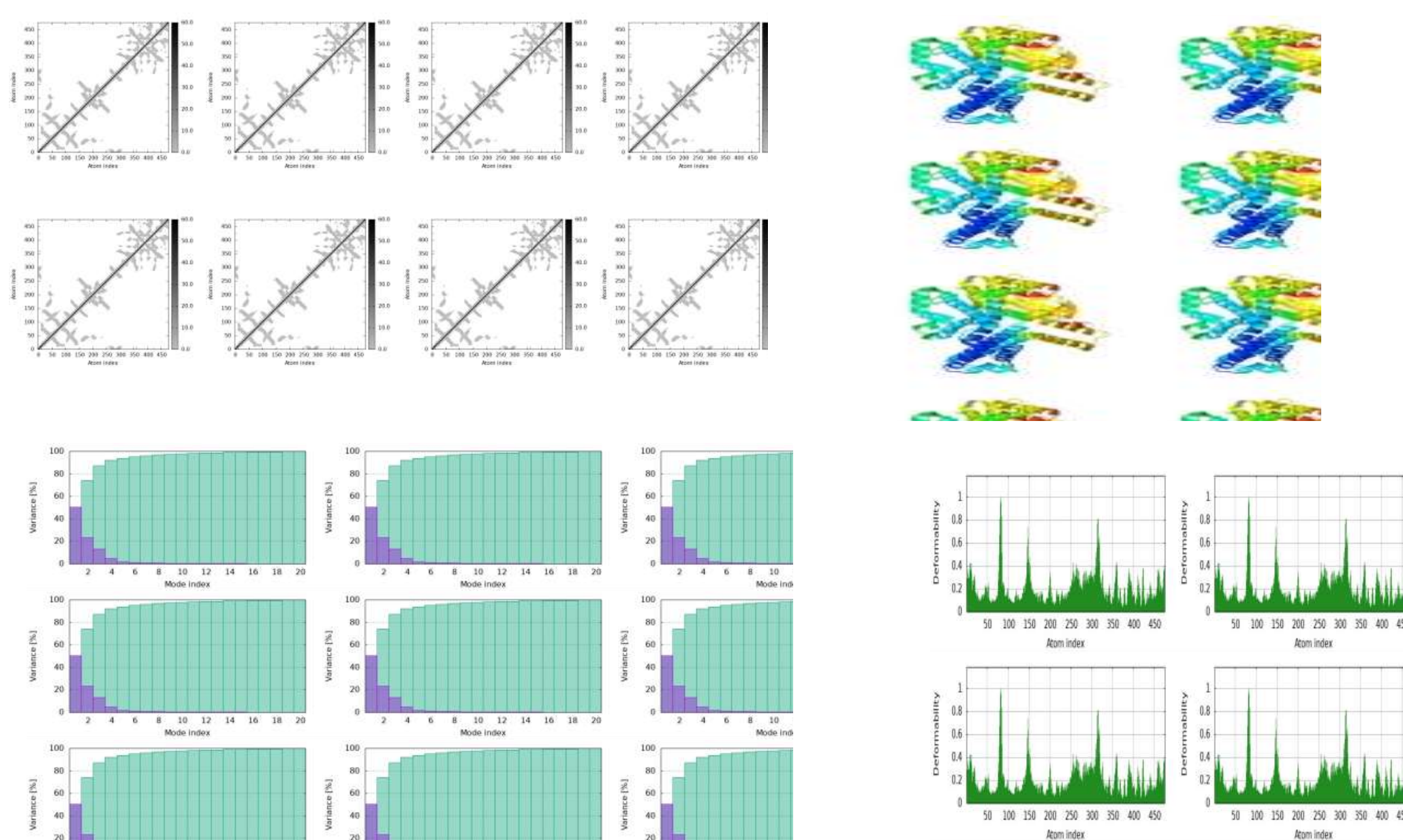
Moreover, we identified important target proteins in the PPI network using the Cytoscape cytohubba plugin. There are eleven computational methods available to Cytohubba, which can examine the key nodes in bioinformatic networks. At the moment, degree method is regarded as being the best method. We discovered in the context of neuro inflammation & inflammation showed high degree values for AKT1, PTGS2, STAT3, PPARG, SIRT1, and MAPK1.



Hub gene network in case of inflammation



Hub gene network in case of neuro inflammation

MD Studies of *Cyamopsis tetragonoloba*

CONCLUSION

According to the results of network pharmacology analysis, in the context of neuro inflammation & inflammation may bind to important target proteins such as AKT1, PTGS2, STAT3, PPARG, SIRT1, and MAPK1. This study raises the possibility that the chemical constituents of this plant might serve as the basis for the development of effective anti-inflammatory and neuro-inflammatory medicine for the treatment of a variety of illnesses, including cancer, neurological disorders, ageing, and rheumatic diseases.

REFERENCES

- ✓ Xanthopoulou, M. N.; Nomikos, T.; Fragopoulou, E.; Antonopoulou, S. Antioxidant and Lipoxigenase Inhibitory Activities of Pumpkin Seed Extracts. *Food Res. Int.* 2009, 42 (5), 641–646. <https://doi.org/10.1016/j.foodres.2009.02.003>.
- ✓ Marie-Magdeleine, C.; Hoste, H.; Mahieu, M.; Varo, H.; Archimede, H. In Vitro Effects of Cucurbita Moschata Seed Extracts on Haemonchus Contortus. *Vet. Parasitol.* 2009, 161 (1–2), 99–105. <https://doi.org/10.1016/j.vetpar.2008.12.008>.
- ✓ Sangeetha G, Vidhya R. In vitro anti-inflammatory activity of different parts of Pedalium murex (L.). *inflammation*. 2016;4(3):31–6.
- ✓ Mohamed Saleem TS, Madhusudhana Chetty C, Ramkanth SV, Rajan VS, Mahesh Kumar K, Gauthaman K. Hepatoprotective herbs—a review. *International Journal of Research in Pharmaceutical Sciences*. 2010;1(1):1–5.
- ✓ Stickel F, Schuppan D. Herbal medicine in the treatment of liver diseases. *Digestive and liver disease*. 2007 Apr 1;39(4):293–304.