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In silico evaluation of the potential for the rational use of garlic and onion crop residue extracts in cosmetics

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INTRODUCTION & AIM

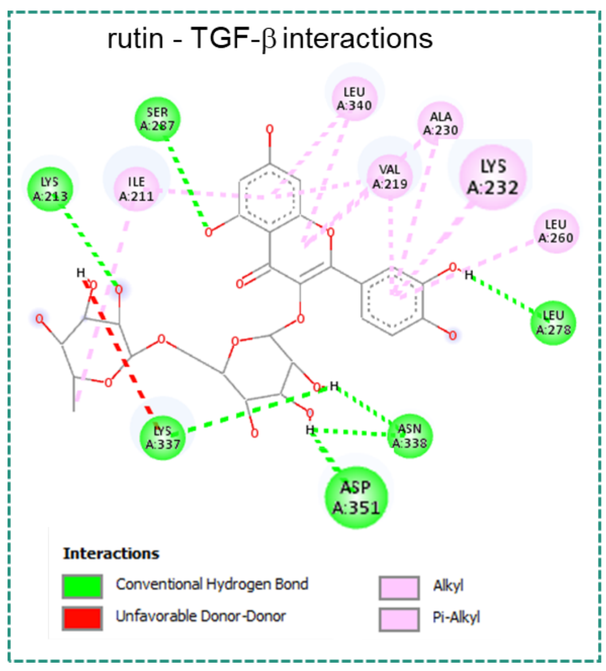
Global environmental issues related to industrial food processing increases the need to recycle biodegradable waste, crop residue or crop by-products and process these natural raw materials for the development of value-added products [1,2]. Notably, an onion and garlic are known for their use in numerous therapeutic and medicinal purposes [3], that also can have a potential use in cosmetic formulations [1]. Nevertheless, developing cosmetic products can be a time-consuming and expensive process. Hence, *in silico* experiments offer a cost-effective and efficient way to investigate the therapeutic potential of natural products. Our molecular docking study explores a potential of molecules identified in garlic/onion extracts to interact with selected proteins (SIRT1, TGF-β and elastase) known to be involved in skin ageing process. Additionally, potential adverse skin effects of each molecule identified in extracts of garlic and onion were evaluated using databases and web tools for skin sensitization tests.

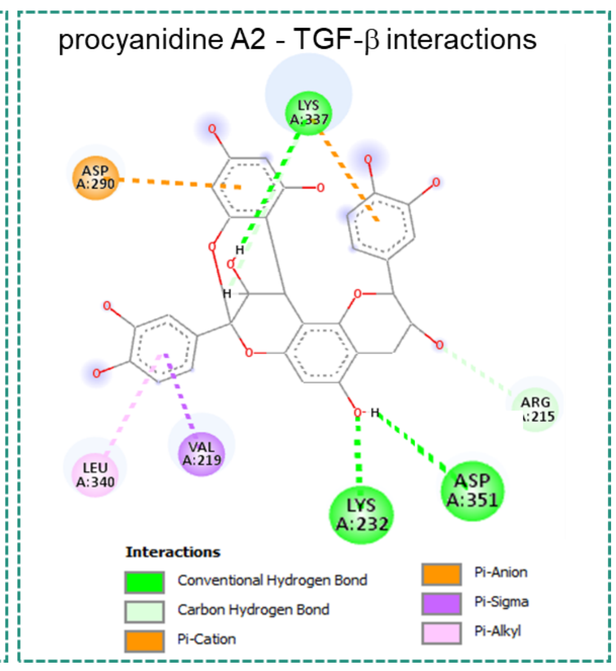
METHOD

The three-dimensional structures of elastase (PDB ID: 1ELB), SIRT1 (PDB ID: 4I5I), and TGF-β (PDB ID: 1vjy) were downloaded from the RCSB Protein Data Bank. The isomeric SMILES strings of selected compounds found in extracts of garlic and onion (unpublished results) were obtained from the PubChem database and were converted into mol2 format using VEGA ZZ 3.2.3. Virtual screening studies were executed by AutoDock Vina software with VegaZZ software as graphical user interface. The crystalized ligand of each protein structure was used to define the docking site. The dimensions of the grid box size were equally set to 24 Å for all three proteins. The grid centers (x, y, and z) coordinates had the following values: (a) 40, 22, and 38 (elastase), (b) 43, -21, and 20 (SIRT1), and (c) 16, 68, and 6 (TGF-β). The exhaustiveness value was set to 50, while the binding modes value was set to 5. All screened compounds were ranked by binding energy (in kcal/mol) based on the AutoDock Vina scoring function (a more negative value indicates higher binding affinity).

RESULTS & DISCUSSION

The molecular docking results showed that rutin and procyanidine A2 have higher binding affinity against TGF-β (-10.8 and -9.5 kcal/mol, respectively) and elastase (-7.9 and -8.3 kcal/mol, respectively), while against SIRT1 exhibited very low binding scores (–4.7 and 16.4 kcal/mol, respectively) compared to the other compounds.





Herein, we report 2D representations of the most favourable binding pose of rutin and procyanidin A2 on the TGF-β catalytic domain, since the binding affinity to this protein showed the best results. The interactions with amino acid residues (Lys232, Asp351) in the enzyme binding pocket that have already been indicated as most important in the crystal structure of the inhibitor [4], were observed in our study. Therefore, our preliminary in silico calculations provide promising results which may be beneficial in the development of skincare products. Web tools for skin sensitization tests of most potent molecules showed no side effects on the skin.

CONCLUSION

Preliminary results indicate that molecules identified in garlic/onion crop residue extracts have a potential to act as inhibitors, allowing possible use of extracts in preparations of skincare products with synergistic anti-ageing action.

FUTURE WORK / REFERENCES

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