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Innovative method to identify antidiabetic plant ingredients as protein tyrosine phosphatase 1B inhibitors

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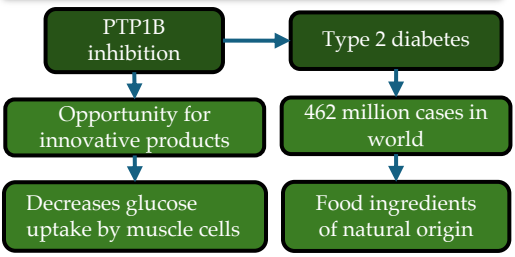
Abstract

There is no disputing the huge costs involved in screening plants as a source of functional ingredients, from extracting compounds to evaluating their biological activity (SDGs 7 and 13). In this context, *in silico* tools are valuable for identifying natural compounds with greater potential for use in the food and pharmaceutical industry. This work aims to use the DiaNat-DB, a database of known antidiabetic compounds from medicinal plants [1], and perform a virtual screening analysis using human Protein Tyrosine Phosphatase (PTP1B) as the protein target. PTP1B inhibition is a promising mechanism in treating type 2 diabetes because its inhibition is related to insulin sensitivity improvement and, consequently, glycemic control. The *in silico* virtual screening methodology was performed using GOLD software for molecular docking and PLP scoring function. Currently, the DiaNat-DB database consists of 360 antidiabetic compounds from 211 plants [1].

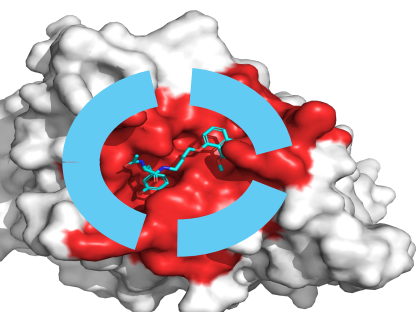
Contextualization of the theme



Framework of the project in sustainability

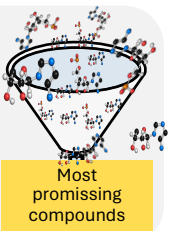
Reuse	Identify Plants with Bioactivities
Reduce	Costs in identifying new ingredients
Innovate	Antidiabetic Ingredients

Figure 1. Protein Tyrosine Phosphatase 1B coupled with selective inhibitor



Methods

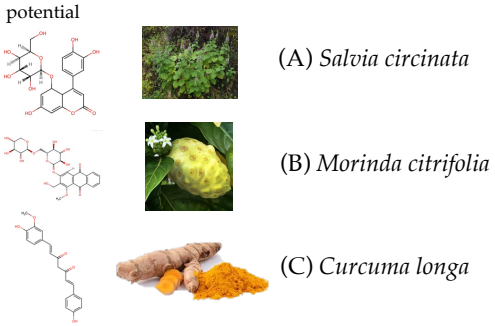
1. Human PTP1b protein selection
2. Protein preparation for molecular modeling
3. Database preparation in DataWarior and Openbabel
4. Virtual Screening and Results Analysis



Conclusion

From the virtual screening analysis performed, three compounds from the DiaNat-DB presented the best predicted inhibition activity: 6,6'',3'''-trihydroxy-7,3',7''-O-trimethylloniflavone, Damnacanthol-3-O-beta-D-primeveroside and Demethoxycurcumin with significant PLP scores of -69,00, -63,56 and -63,30, respectively. The PLP scores compared well with the PLP score obtained for Sulfamic Acid (-34,30), the control compound used in this study. These compounds were found in the plant species: (A) *Salvia circinata*, (B) *Morinda citrifolia* and (C) *Curcuma longa*, respectively. This study presents an innovative method for identifying molecules and plants with potential antidiabetic activity as functional ingredients for the food and pharmaceutical industry.

Figure 2. Natural compounds with antidiabetic potential



References

[1] Madariaga-Mazón A, Naveja JJ, Medina-Franco JL, Noriega-Colima KO, Martinez-Mayorga K. DiaNat-DB: a molecular database of antidiabetic compounds from medicinal plants. RSC Adv. 2021 Jan 28;11(9):5172-5178

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