

# In Vitro Study on Pancreatic Lipase to Reduce Obesity through Molecular Docking

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## DESCRIPTION

Obesity is a major public health issue which keeps growing faster. Reducing the amount of energy consumed through a method that acts through intestinal absorption is one of the most crucial therapy strategies. Therefore, an enzyme called Pancreatic Lipase (PL) hydrolyzes dietary triglycerides that are consumed from meals. Due to the fact that dietary fats are the main source of lipids, after being absorbed in the intestines, fat molecules are transformed into Triglycerides (TG), which are then stored in the body as a primary source of energy. Therefore, by focusing on the enzyme PL, intake of high levels of dietary fats that contribute to a rise in triglyceride intake can be decreased.

PL is a crucial enzyme that aids in the breakdown of dietary fats, hydrolyzing 56% of them. The pancreas secretes a protein called PLRP1, which has no known activities. Although PLRP1 is secreted into the duodenum and shares a high degree of homology (68%) with PL, no evidence of lipolytic activity (the breakdown of TGs) has been found. The fact that the PLRP1 protein has two site-directed amino acids that are also present in PL and that may be the cause of the lipolytic activity suggests that it may be a non-functional homologue. Additionally, PLRP1 and PLRP2 are primarily expressed during the suckling phase, whereas PL is primarily expressed after adulthood, indicating a physiological distinction that is not fully understood.

According to earlier reports, PLRP1 uses as a cDNA probe to analyse the dietary TGs. When Lowe first replicated the PL, Wicker-Plan quart and Puig server referred to it as the "rat PL." The total number of TGs discovered and reported in rats, found in both PL and PLRP1. The reports indicated higher PLRP1 levels, but there is currently no documented scientific proof to support the proof of concept. One of the finest methods for realising this idea of lipid digestion towards PLRP1 is determining its activity through virtual high throughput screening.

Orlistat is the only traditional medication for the treatment of obesity that is approved by the FDA. It is utilised as a non-specific PL inhibitor. Therefore, recent strategies for combating lipase inhibitors have generated interest in natural product sources, which might not have some of the negative effects that have been documented. Inhibiting the PL, which is in charge of lipid metabolism, is one method of employing natural compounds to reduce the absorption of dietary lipids.

Plant based medications have become more important in obesity treatment plans. The identification of additional targets to fight obesity is intriguing when considering molecules produced from plant sources. Now a days natural products are increasing interest for treating obesity and may also contribute to the development of cholesterol lowering medications due to their low cost and unfavourable side effects induced by those synthetic therapies. Molecules from natural sources frequently have more drug-like characteristics in their structural ranges, making them more receptive to administration into the body. There are numerous plants that are said to hydrolyze lipids. Our current area of interest in the search for compounds from natural sources primarily focuses on the families of polyphenols, primarily flavonoids, that are believed to be PL inhibitors.

Using screening based on computational approaches is currently one of the main strategies to successfully identify the newer drug targets from natural sources. The use of Computer Aided Drug Discovery (CADD) methods, including ligand and structure-based virtual screening using docking software, has been shown to be particularly effective in identifying novel hit compounds for the targets, resulting in the successful discovery and development of new drugs. Therefore, a similar strategy concentrating on computational models, such as molecular docking, was used to identify effective PLRP1 inhibitors. To the best of our knowledge, PLRP1's impact on lipid digestion hasn't been previously documented. Thus, by screening reported flavonoid compounds, our primary objective is to identify the PL inhibitors by targeting the 2PPL protein, also known as PLRP1.

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