Therasyn: In silico Design and Multi-Scale Simulation of a Targeted Oral Combination Drug for Alpha-1 Antitrypsin Deficiency Related to Chronic Obstructive Pulmonary Disease

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Alpha-1 antitrypsin deficiency (AATD) is a genetic disorder that can lead to chronic obstructive pulmonary disease (COPD), a progressive lung condition that causes breathing difficulty. AATD limits the body's ability to control lung inflammation and repair tissue damage. Current treatments are expensive and do not effectively reach damaged areas in the lungs. In my project I developed Therasyn, a new combination pill made of three natural compounds—caprylic acid, bromelain, and sulforaphane—designed to reduce inflammation and support lung repair by increasing the activity of a gene called TLE1, which plays a role in immune regulation. The drug was developed and tested entirely through computational simulations. Molecular docking (a simulation that predicts how molecules fit together like puzzle pieces) showed that Therasyn binds strongly to the TLE1 protein. Further modeling showed that the protein stays structurally stable after the drug binds to it, which is essential for the treatment to work properly. A 3D simulation of airflow (called computational fluid dynamics) was used on COPD-damaged lungs, and showed improved breathing patterns when Therasyn was applied. Therasyn was also designed as a pill with a dual-layer coating that only dissolves under certain pH conditions in the body. Simulations of how the drug spreads and breaks down (called pharmacokinetic and diffusion modeling) showed it releases at the right time and stays active long enough to be effective. Finally, a virtual safety test (ADMET analysis) predicted that Therasyn is safe, absorbable, and well-tolerated. By combining natural ingredients with multiple beneficial effects, Therasyn offers a promising oral treatment for AATD-related COPD.

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