

## Computational Elucidation of $\beta$ -endo-Acetylglucosaminidase (LytB) Inhibition by Kaempferol, Apigenin, and Quercetin in Streptococcus pneumoniae: Anti-Pneumonia Mechanism

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**Abstract :** Reviewers' Comments: The study provides valuable insights into the anti-pneumonia properties of flavonoids against LytB. Authors could further validate findings through in vitro studies and consider exploring combination therapies for enhanced efficacy. Response: Thankyou for your valuable comments. This study has been conducted further via experimental validation of the in-silico findings. The study uses Streptococcus pneumoniae D39 strain and examine the anti-pneumonia effect of kaempferol, quercetin and apigenin at various concentrations ranging from 9ug/ml to 200ug/ml. From results, it can be concluded that the kaempferol has shown the highest cytotoxic effect (72.1% of inhibition) against S. pneumoniae at concentration of 40ug/ml compare to apigenin and quercetin. The treatment of S. pneumoniae with concoction of kaempferol, quercetin and apigenin has also been performed, it is noted that conc. of 200ug/ml was most effect in achieving 75% inhibition. As S. pneumoniae D39 is a virulent encapsulated strain, the capsule interferes with the uptake of large size drug formulation. For instance, S. pneumoniae D39 with kaempferol and gold nano urchin (GNU) formulation, but the large size of GNU has resulted in reduced cytotoxic effect of kaempferol (27%). To achieve near 100% cytotoxic effect on the MDR S. pneumoniae D39 strain, the study will target the development of kaempferol-engineered gold nano-urchin' conjugates, where gold nanocrystal will be of small size (less than or equal to 5nm) and decorated with hydroxyl, sulfhydryl, carboxyl, amine and groups. This approach is expected to enhance the anti-pneumonia effect of kaempferol (polyhydroxylated flavonoid). The study will also examine the interactive study among lung epithelial cell line (A549), kaempferol-engineered gold nano urchins, and S. pneumoniae for exploring the colonization, invasion, and biofilm formation of S. pneumoniae on A549 cells resembling the upper respiratory surface of humans.

**Keywords :** streptococcus pneumoniae,  $\beta$ -endo-Acetylglucosaminidase, apigenin, quercetin kaempferol, molecular dynamic simulation, interactome study and GROMACS

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