Graduate School of Science and Technology Master's Thesis Abstract

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Abstract

The global pandemic, COVID-19, caused by the SARS-CoV-2 virus, has precipitated an urgent search for effective therapeutic interventions. In response to this, our research aimed to identify natural compounds with potential inhibitory effects on the entry of the SARS-CoV-2 Spike (S) glycoprotein into host cells. Utilizing the PDBJ and BindingDB databases, we isolated 204 S glycoprotein sequences and identified 33,722 binding molecules respectively, using clustering analysis and the BLASTp method. These molecules were subsequently compared with 51,678 secondary metabolites from the KNApSAcK database to identify potential inhibitors.

After discarding metabolites of unknown origin and conducting docking analyses, several secondary metabolites emerged as potential drug candidates based on their docking and SwissADME bioavailability scores. Myristoleic acid and cis-10-Pentadecenoic acid showed promise for inhibiting cluster 1 of the SARS-CoV-2 Spike protein, Colchamine (Demecolcine) for cluster 2, and multiple metabolites including C00000218, C00000446, C00002035, C00017543, C00027661, and C00036384 for cluster 4. Our findings lay the groundwork for further experimental validation of these compounds as therapeutic agents against SARS-CoV-2.