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Interactions between SARS-CoV-2 spike fragment and ACE2-derived peptides or peptide-decorated liposomes

The severe acute respiratory syndrome coronavirus type 2 (SARS-CoV-2), which causes the coronavirus disease 2019 (COVID-19) still poses a real threat to human health and challenges worldwide healthcare systems. Despite numerous mutations in the spike of SARS-CoV-2, which raise concerns about escape from vaccines and therapeutic drugs, the essential mechanism for virus infection remains unchanged –the viral spike protein binds to the angiotensin-converting enzyme II (ACE2). One of the strategies to inhibit the SARS-CoV-2 infection is a neutralisation of the virus before it enters human cells.

In our project, we explored the interactions of ACE2-derived peptides with the spike receptor binding domain (S-RBD) of SARS-CoV-2. Interaction studies between peptides and S-RBD were performed in silico and with microscale thermophoresis (MST). Based on molecular dynamics studies binding energies of several peptides and S-RBD were calculated. MST experiments revealed significant differences in the half-maximal effective concentration (EC50) of peptides. Two of the designed peptides were used in further experiments. Peptide-decorated liposomes were synthesized with the use of the selected peptides and then studies of their interactions with S-RBD were performed. Based on the results of MST studies we concluded, that the synthesized peptide-decorated liposomes interact with S-RBD and may be potentially used as SARS-CoV-2 inhibitors.

Our studies demonstrate, that ACE2-derived peptides and peptide-decorated liposomes interact with S-RBD, which shows their possible application as new anti-SARS-CoV-2 agents. Nanotherapeutics based on the structure of naturally occurring proteins seem a promising tool in a devising of novel antiviral strategies.

References

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