In silico approaches to drug repositioning for COVID-19 at AMED-BINDS

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In silico prediction based on the protein structures of SARS-CoV2 is effective to find the putative drug candidates from the approved drugs, as drug repositioning. The main protease, 3CL protease, of SARS-Cov2 is essential for proteolytic maturation of the virus, and inhibiting its function could prevent the COVID-19 spreading. Here, recent activities in the in-silico unit of AMED-BINDS are introduced.

Hirokawa et al. adopted an *in silico* docking-based screening approach, which combines molecular docking with a protein-ligand interaction fingerprint (PLIF) scoring method, utilizing the crystal structure of SARS-Cov2 3CL protease (PDB: 6LU7) and a database of known drugs (KEGG-Drug). Selected drugs have the binding modes similar to PLIF of the known active N3 inhibitors with favorable docking scores. They identified one hundred and several dozen potentially candidate drugs for 3CL protease inhibitors, which are already approved as antiviral, HIV protease inhibitors, antibacterial or antineoplastic agents.

Sekijima et al. analyzed the interactions between 3CL protease and the drug candidate compounds using molecular dynamics simulation. Through this study, they aim to elucidate the interactions between 3CL protease and the drugs.

The chemical compound libraries in AMED-BINDS will also be available in the future assay studies.