

Exploring new drug candidates for COVID-19 by "Fugaku"

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Research content:

Currently, clinical trials are underway in Japan and overseas to confirm the effects of existing drugs on COVID-19. Some reports have shown that the drug has shown efficacy through these clinical trials, but the number of cases has been small, and no effective therapeutic drug has yet been identified. Furthermore, due to the small number of drugs being tested, it is possible that none of the drugs have a definite effect.

Therefore, in this study, we performe molecular dynamics calculations using "Fugaku" to search and identify therapeutic drug candidates showing high affinity for the target proteins of COVID-19 from approximately 2,000 existing drugs that are not limited to existing antiviral drugs targeted in clinical trials.

Expected results:

- ✓ New therapeutic drug candidates other than those currently undergoing clinical trials can be discovered.
- ✓ Combination effects of multiple drugs can be estimated
- ✓ The molecular action mechanism of existing drugs currently undergoing clinical trials will be elucidated. In addition, these findings provide a clear direction for developing new drugs that go beyond the existing drugs.

