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Dynamic Residue Interaction Network Analysis of Secondary Mutations in Protease that Promote Drug Resistance in HIV-1

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The human immunodeficiency virus (HIV) is the pathogen of the Acquired Immune Deficiency Syndrome (AIDS). AIDS has become a disease that can be controlled in the long term by anti-HIV drugs. However, there are serious concerns about the emergence of viral mutants that are resistant to anti-HIV drugs. Some amino acid mutations in HIV-1 protease promotes development of drug resistance caused by primary mutations, even without directly affecting drug efficacy against anti-HIV drugs. These mutations are referred to as "secondary mutations". In this study, we investigated the dynamic correlation between the drug binding site and its secondary mutation site in HIV-1 protease using dynamic residue interaction network (dRIN) analysis [1] based on molecular dynamics simulations.

[1] Yadav, M., Igarashi, M., Yamamoto, N.; Dynamic residue interaction network analysis of the oseltamivir binding site of N1 neuraminidase and its H274Y mutation site conferring drug resistance in influenza A virus, *PeerJ*, **2021**, *9*, e11552.