# Understanding of binding molecular mechanism of hemagglutinin H3N2 of influenza virus complexed with arbidol and derivatives: A molecular dynamics simulation perspective

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Recently, the H3N2 influenza outbreak has caused the serious global public health concern for the next influenza pandemic control. Since using of current anti-influenza drugs targeting on neuraminidase (oseltamivir and zanamivir) and the proton M2 channel (amantadine and rimantadine) leads to drug resistance, it is essential to seek for new anti-viral agents that act on additional viral targets. Hemagglutinin, a glycoprotein embedded in the viral surface and playing a critical role in influenza viral replication cycle has become as attractive target. This work investigates the binding molecular mechanism of hemagglutinin H3N2 of influenza virus complexed with arbidol and its derivatives by means of molecular dynamics simulation. The result showed that arbidol derivatives could form strong hydrogen bonds with surrounding amino acids such as THR59 (HA2), ASP90 (HA2), LYS307 (HA2), GLU103 (HA2), LYS58 (HA2) and ASN60 (HA2), while arbidol is not able to make this kind of interaction. Moreover, the binding free energy prediction is in agreement with experimental data indicating that derivative compounds show high potency against hemagglutinin H3N2. Detailed information is very helpful for further design and optimize hemagglutinin inhibitors with high efficiency.

## References

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