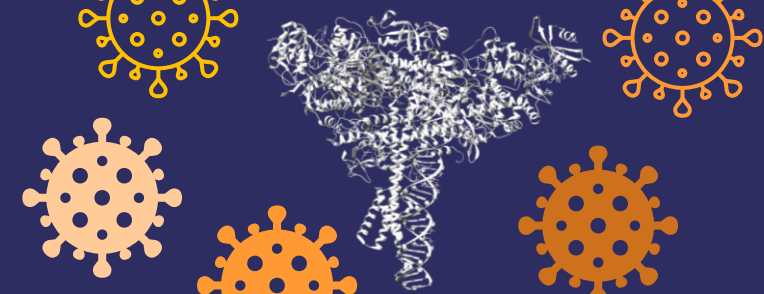# The RNA Helicase Protein

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What is it?

The RNA helicase protein (**NSP13**) is important for the survival of the SARS-CoV-2 virus, making it a key **target** for antiviral drugs. However, many drugs targeting the coronaviral helicase can also damage **human** proteins as they are not **selective** enough. This research aimed to look at the structure and movement of NSP13, which would be useful for **specific** inhibitor design.

What was done?

HECBioSim coordinated a community response, backed with resources and **support** by directing academics into multi-institutional and multidisciplinary teams. They also provided high performance computers for multi-resolution analysis of NSP13.
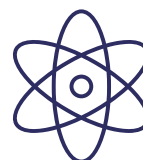
Molecular dynamics simulations and **structural analyses** were performed on NSP13 by the research team to provide key insight into the structure, machinery and potential inhibitor targets of the protein.
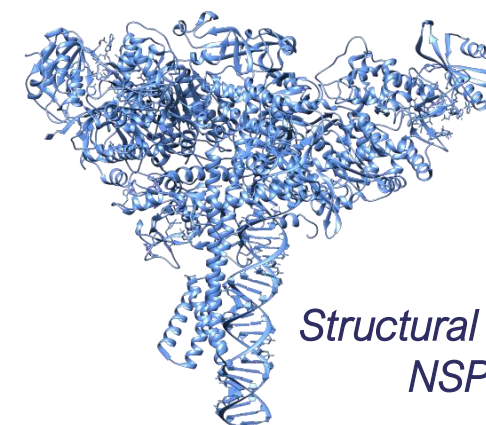
Structural model of NSP13

Using powerful computers, researchers were able to rapidly gain insight into the mechanism behind viral replication.

What was found?

Some key findings include:

- NSP13's genetic sequence is **≤20% similar** to proteins outside the *Coronaviridae* family, which is important knowledge for designing new drugs for **mutating** viruses
- The **specific mechanism** NSP13 uses to aid in viral **replication**
- How NSP13 **interacts** with other molecules bound to it
- The **movements** of NSP13 and what induces them

These findings provide a solid basis for future research looking at making antivirals specific to the SARS-CoV-2 virus that do not destroy human proteins.

Reference| Berta, D., Badaoui, M., Martino, S.A., Buigues, P.J., Pisliakov, A.V., Elghobashi-Meinhardt, N., Wells, G., Harris, S.A., Frezza, E. and Rosta E. (2011). Modelling the active SARS-CoV-2 helicase complex as a basis for structure-based inhibitor design. *Chemical Science,* [online] 12(40), pp.13492-13505. doi:10.1039/D1SC02775A