Supplementary Information

Supplemental data 1. The quality criteria of the NS3/4A models.
**Supplemental data 2.** Top five clusters of interaction between the modeled NS3/4A and nanobody provided by the server

Graphical representations of the HADDOCK-clone V₁H24

Clusters of NS3/4A-V₁H₂₄

Cluster 1

Cluster 6

Cluster 8

Cluster 4

Cluster 3
Graphical representations of the HADDOCK-clone VH28

Clusters of NS3/4A-VH28

Cluster 3
Cluster 4
Cluster 2
Cluster 8
Cluster 6
Graphical representations of the HADDOCK- clone V_{H}H41

Clusters of NS3/4A-VH_{H}41

Cluster 5

Cluster 1

Cluster 8

Cluster 6

Cluster 11
**Supplemental data 3.** Modeled structure of NS3/4A showing catalytic triad, oxyanion loop and S1 pocket.