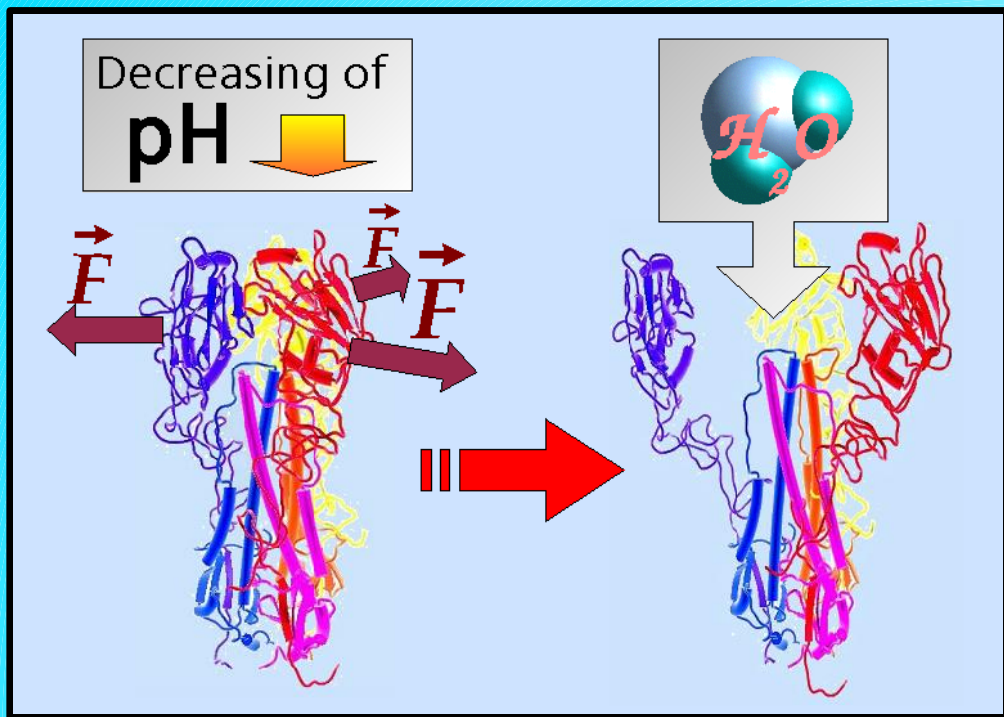


*Role of the water molecules in the structure and function of*  
**viral protein and virus infectivity.**

Shepelenko S. O., Salnikov A. S., Rak S. V., Goncharova E. P., Ryzhikov A. B.

**Federal State Research Institution - State Research Center of Virology and  
Biotechnology "Vector"  
of the Federal Service for Surveillance on Consumer Rights Protection and Human  
Well-being,  
Koltsovo, Novosibirsk Region, Russia.  
Novosibirsk State University,  
Pirogova Street 2, Novosibirsk, Russia.**

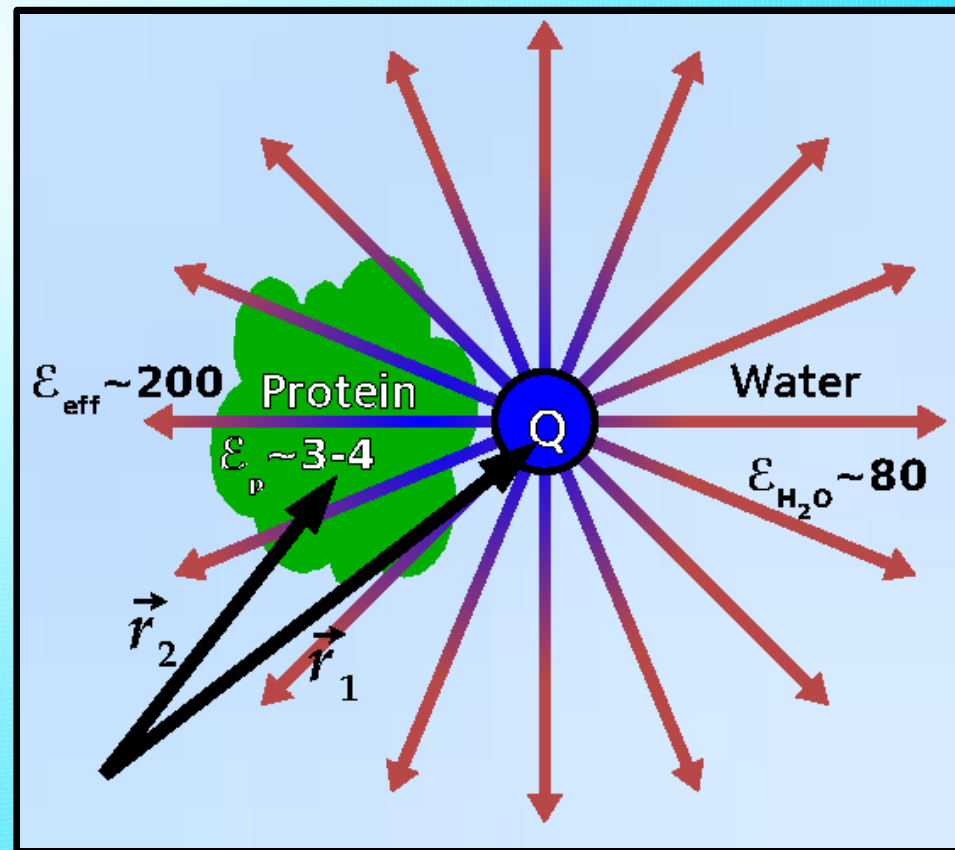


$$\vec{E}(\vec{r}_0) = \vec{E}_Q(\vec{r}_0 - \vec{r}_1) + \vec{E}_{\text{polarization}}(\vec{r}_0, \vec{r}_1, \vec{r}_2);$$

effects

$$E_Q = \frac{Q}{\epsilon_{H_2O} \cdot r^2}, \quad \vec{r} = \vec{r}_0 - \vec{r}_1;$$

$$E = \frac{Q}{\epsilon(\vec{r}_1, \vec{r}_2) \cdot r^2}$$



## Results

- ✓The physical model for calculation of polarization effects for protein interactions was developed.
- ✓The role of water molecules in the setting of threshold value of repulsive forces of hemagglutinin protein domains at the trigger stage of conformational changes was shown.
- ✓Kinetics of virus-induced hemolysis for different influenza virus strain was experimentally measured.
- ✓Trigger pH values for different influenza virus were both calculated with help of the program and measured experimentally.