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Biothermodynamics of virus-host interactions: The role of Gibbs energy in antigen-receptor binding and virus multiplication in host cells

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SUMMARY

- Viruses overtake nutrients from host cells due to more negative Gibbs energy.
- Mechanistic model of virus-host interactions based on nonequilibrium thermodynamics was developed.
- Virus evolution can be analyzed with the methodology of biothermodynamics.

INTRODUCTION

- Viruses are complex macromolecular assemblies that interact with their host organisms.
- Virus-host interactions are processes that proceed in accordance with the laws of physics and chemistry.
- Biothermodynamics studies biological structures and processes with the methodology of chemical and nonequilibrium thermodynamics.
- Biothermodynamics has been applied in science and engineering to analyze microorganisms, which include bacteria, yeasts, filamentous fungi and algae.
- In this research, the approach of biothermodynamics was applied to study virus-host interactions and virus evolution.

METHODS

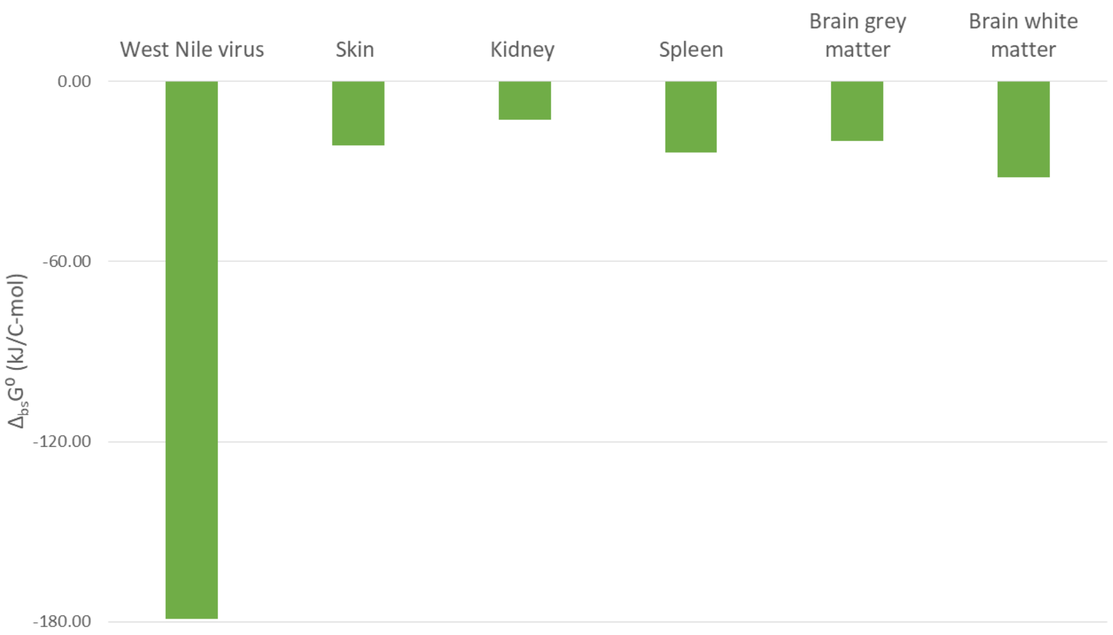
- Atom counting method was applied to calculate empirical formulas of viruses, based on their genetic sequences, protein sequences and morphology.
- Patel-Erickson-Battley model was used to find enthalpies, entropies and Gibbs energies of virus particles, based on their empirical formulas.
- Biosynthesis reactions of viruses were formulated, based on empirical formulas, with the rules of stoichiometry.
- Thermodynamic properties of biosynthesis of viruses were calculated with the methodology of thermochemistry.

VIRUS-HOST INTERACTIONS

- Gibbs energy is the driving force of metabolism and multiplication of microorganisms, including viruses.
- Phenomenological equations belong to nonequilibrium thermodynamics and relate rates of processes and their driving forces.
- Biosynthesis phenomenological equation shows how Gibbs energy of biosynthesis, $\Delta_{bs}G$, determines biosynthesis rate, r_{bs}

$$r_{bs} = -(constant) \cdot \Delta_{bs}G$$

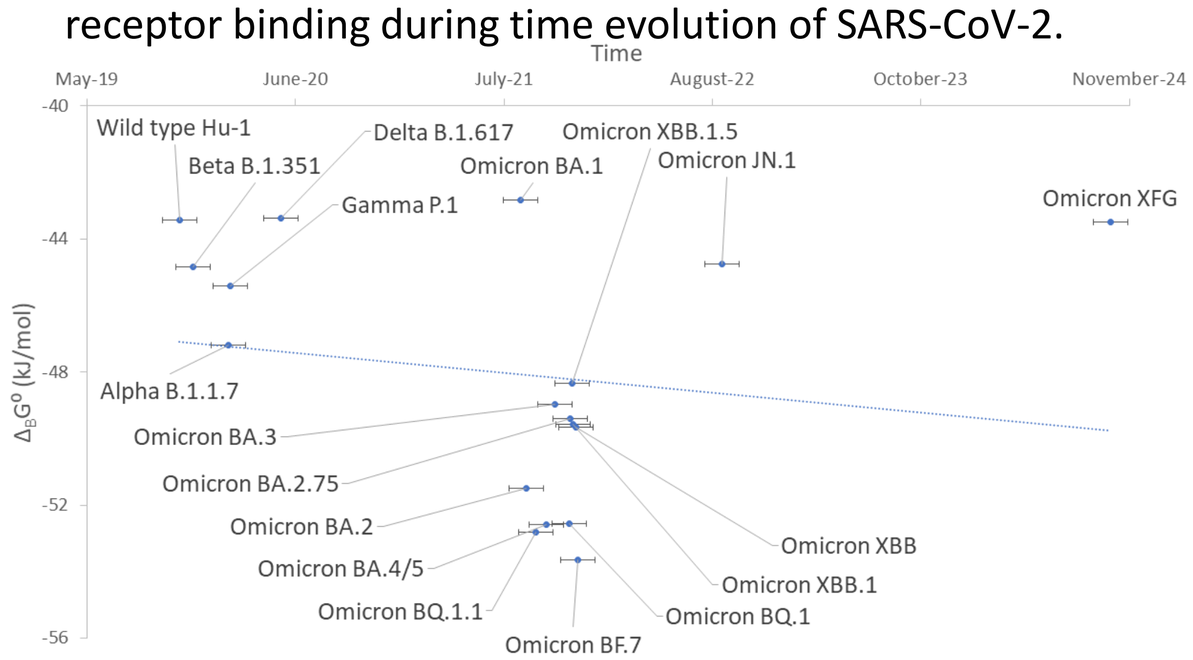
- Figure 1 shows Gibbs energies of biosynthesis of a virus and its host tissues.



- The virus has a more negative Gibbs energy of biosynthesis than its host tissues.
- More negative Gibbs energy leads to greater biosynthesis rate of the virus, due to the phenomenological equation.
- The host cell metabolic machinery will produce more virus components that host cell binding blocks.
- In this way the virus hijacks the host cell metabolic machinery

VIRUS EVOLUTION

- Figure 2 shows driving force (Gibbs energy) of antigen-receptor binding during time evolution of SARS-CoV-2.



- SARS-CoV-2 is evolving towards decreased pathogenicity and increased infectivity, in agreement with the evolution theory.

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