bly of artificial vRNPs formed by PVX CP and different plant and animal RNAs. To obtain data about the particles size (hydrodynamic diameter) and concentration the method of Nanoparticle Tracking Analysis (NTA) was used. PVX CP was incubated with PVX RNA and different viral RNAs. Formed cognate and artificial vRNP were analyzed by NTA. This method based on laser-illuminated optical microscopy enables to detect the RNPs assembly in real-time in liquid. The detected number of formed particles indicates the assembly efficiency. For the first time the information about efficiency of the potato virus X particles assembly was obtained by NTA. The assembly efficiency of RNPs formed by PVX CP with PVX RNA and heterologous viruses RNA was compared. The proposed method allows studying the mechanisms of initiation and elongation of the viral ribonucleoproteins.

Reference

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Keywords: assembly, plant virus, ribonucleoprotein.

WED-016
Computer simulation method to generate the variant sequences of influenza viruses using the time series substitution pattern

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Since the outbreak of novel influenza pandemic in 2009, various kinds of simulation methods have been developed. Most of the developments, however, are focused on the determination of the spreading patterns of influenza viruses over time. In this study, we introduce a novel approach to predict the possible variants of influenza viruses using the empirical data of nucleotide sequences determined by experimental methods. We developed a simulation tool named SimFlu (simulation tool for influenza virus) to predict possible future variants of influenza viruses. SimFlu can create variants from a seed nucleotide sequence of influenza A virus using the codon variation parameters included in the SimFlu package. The SimFlu's library provides pre-calculated codon variation parameters for H1N1, H3N2 and H5N1 subtypes of influenza A virus isolated from 2000 to 2011. All the source sequences (56 328 sequences) of the SimFlu's library were collected from the Influenza Virus Resources at NCBI. The SimFlu supports 3 types of operating systems, including Windows, Linux, and Mac OS X, and it also provides a command option-based version to run on a Linux queuing system. SimFlu is publicly available at http://lcbb.snu.ac.kr/simflu. Moreover, we also developed an analytical tool for calculating the codon substitution patterns named SimFluVar to support the researchers who want to use their own variation parameters. SimFluVar provides precise patterns of co-don variations between 2 viral groups, especially for the influenza virus groups. SimFluVar also provides the useful functions, such as editing and visualization of the result matrix. SimFluVar is in C++, and Java RCP is used for distribution package. Documentation, examples, results and source code are available at http://lcbb.snu.ac.kr/simfluvar.

Keywords: codon variation, computer simulation, INFLUENZA VIRUS.

WED-017
Conformational flexibility and domain binding interfaces in human tyrosyl-tRNA synthetase studied by molecular dynamics simulations

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Human tyrosyl-tRNA synthetase (*Hs*TyrRS) is a key enzyme of protein biosynthesis, which catalyzes the aminoacylation of cognate $tRNA^{Tyr}$ and also reveals non-canonical cytokine activities. After proteolytic cleavage *Hs*TyrRS reveals both IL8-like activity of its N-terminal catalytic module and EMAP II-like activity of non-catalytic C-terminal domain (Wakasugi and Schimmel, 1999; Kornelyuk et al., 1999). Earlier, it was found that the ELR-motif (E91, L92, R93) in *Hs*TyrRS is responsible for IL8-like cytokine activity (Wakasugi and Schimmel, 1999), but its structural state in full-length human TyrRS was unknown.

In this work we constructed the model of the full-length *Hs*TyrRS structure and studied its putative compactization by all-atom molecular dynamics simulations. All MD computations were performed using grid services of the MolDynGrid virtual laboratory (http://moldyngrid.org). 3D structure of *Hs*TyrRS was constructed in Modeller 9.7 using structure templates (1N3L, 1NTG, and 1OPL for interdomain linker). Six independent 100 ns MD trajectories of *Hs*TyrRS were computed using GROMACS 4.0.5 software in G43a1 force field. The Contacts Analyzer Script (CAS) and the tRMSF tool of the Pteros molecular modeling library (http://pteros.sourceforge.net) were used for MD simulation data analysis. The Distributed Analyzer Script was used for analytical tools automation (Savytskyi et al., 2011).

Our MD simulations revealed the strong binding energy of ~1000 kJ/mol for C-module binding to mini-TyrRS dimer. Antiparallel β-sheet formation at the Ala355-Val363 region of interdomain linker was observed at 3–100 ns time interval (~85% of time). Also, the β-turn formation at the Pro365-Arg367 region was revealed for 40–90 ns time interval (~50% of time).

During 100 ns MD simulations the H-bonds formation between R93 residue of ELR cytokine motif and A340 and E479 residues of C-module was observed. These findings support the idea that the full-length TyrRS lacks its cytokine activity due to the direct interactions between N-terminal and the C-terminal modules, which protect the ELR cytokine motif.

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Keywords: tyrosyl-tRNA synthetase; cytokine; ELR motif; molecular dynamics; interdomain linker; GROMACS.