MLZ Conference 2021: Neutrons for Life Sciences



Contribution ID: 51

Type: Talk

Integrative approach to structure of huge protein complex in Kai-clock protein system

Wednesday, 9 June 2021 11:10 (20 minutes)

Kai-clock system is one of the simplest biological clocks: the system is composed with only three proteins, KaiA, KaiB and KaiC, and they repeat association-dissociation with 24-hrs period as follows, A2+B4+C6 \rightarrow A2C6+B4 \rightarrow A2+B6C6 \rightarrow A12B6C6 \rightarrow A2+B4+C6 \rightarrow ... To understand this system, it is essential to reveal the complex structures in every phase. For this purpose, we have been focused on the largest complex, A12B6C6, which could appear at the turning point from the association phase to the dissociation phase. Basic structure of A12B6C6 was reported with cryo-EM observation by J. Snijder, et al.. However, the reported structure missed the N-term domains of KaiA. Here, we introduced the whole structural model of A12B6C6 in solution. To analysis this huge complex in solution, we utilized two state-of-art solution scattering techniques, SEC-SAXS and SEC-inversed Contrast Matching-SANS (SEC-iCM-SANS). In addition, we combined computational modeling and molecular dynamics simulation to build three-dimensional structure and to clarify its dynamics. We should note that the iCM-SANS selectively observing the KaiA protomers in the complex played crucial role in the analysis. The detailed will be shown in the presentation.

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