Conformational analysis of trigger factor and its mutant II. DAMMIN analysis

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Introduction
We have studied trigger factor (TF) and its truncated mutants (C419, C360, NM and MC) [1]. SAXS experiments were performed at BL15A with CCD detector. Mutants showed aggregation that was reflected to scattering intensity. Then we use two-exponential equation to analysis as

\[ I(h) = I_1 \exp(-R_g^2 h^2/3) + I_2 \exp(-R_g^2 h^2) \]

where I is intensity, Rg is radius of gyration and h is scattering vector. The smaller Rg gives the Rg of the monomer, while the larger one gives the average Rg of oligomers, if they are well separated (unpublished data). By subtracting oligomers part, we can extract monomer data. Molecular structures were calculated for monomer data by program DAMMIN [2].

Result
Structures are shown in Fig. 1. TF-crystal is from PDB 1w26. MC-crystal and NM-crystal are calculated by omitting domains from TF-crystal.

The structure of TF in solution showed very similar to the crystal structure in shape and size. The structure of C419 in solution is similar to that of TF but slightly different from that of TF. The structure of C360 in solution is clearly different from that of TF. It is composed of two domains with a link part, which is coincident with the results of p(r) function having two peaks [1]. The apparent crystal structure of NM is special. As C-domain, located in the middle of the TF structure, is truncated, the NM crystal forms a “linear” structure. In contrast, NM in solution takes a compact structure. Thus, NM does not take the “linear” structure.

The structure of MC (N-terminal is truncated) in solution remains almost the same structure with the crystal, which suggests the N-terminal does not affect the stability of M and C parts of the protein significantly.

References
[1] Zhou et al. this activity report
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Fig. 1 Structures of TF and its mutants