The vaccinia virus A46 protein comprises 240 a.a. and according to structure predictions has a single globular domain with a short hypothetical unstructured C-terminus. Both A46 alone and a fusion with maltose binding protein (MBP) expression vectors were constructed. Only the fused protein construct was expressed at the sufficient level for further studies. Using TEV proteolysis, we could cleave A46 protein from the MBP-A46 construct. Both MBP-A46 and cleaved A46 protein were purified to homogeneity. The MBP-A46 construct behaved as a dimer where as A46 alone behaved as a tetramer on size exclusion chromatography. A limited proteolysis experiment confirmed the presence of one domain in A46. We set up a number of crystallization screens with A46 protein but failed to obtain any reproducible crystals.

The cellular target of A46 protein is the adaptor protein MyD88, which participates in numerous signal transduction cascades during both innate and acquired immune responses. The MyD88 protein is composed of two domains, including the C-terminal TIR (Toll/IL1-like) domain. According to bioinformatic predictions, the viral A46 protein should contain a TIR fold, similar to MyD88. Thus, the TIR domain in MyD88 is believed to be the site of the interaction between A46 and its target. To test this hypothesis, the C-terminal part of the murine MyD88 protein, comprising the TIR domain (146-296 a.a.), was expressed with a GST-tag and purified. We will now study the A46 and MyD88 interactions via pull-down assays and isothermal titration calorimetry, as well as crystallization of the purified complex.

Keywords: vaccinia, A46, MyD88

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Reorganization of the shell protein during the maturation of bacteriophage T7

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Maturation of dsDNA bacteriophages involves the assembly of the virus prohead from a limited set of structural components followed by rearrangements required to acquire the stability that is necessary for infecting a host under challenging environmental conditions.

Bacteriophage T7 infects *Escherichia coli* and belongs to the Podoviridae family. It has a 40kb dsDNA, an icosahedral capsid with a triangulation number T=7, and a non-contractil tail [1]. The virus shell is made of 415 copies of protein gp10A. The prohead also contains a scaffolding protein (gp9) and a dodecameric connector (gp8) that attaches a core complex to one of the 12 5-fold vertices. The structure of of the T7 prohead and mature head have been solved by three-dimensional cryo-electron microscopy [2], and quasi-atomic models for the procapsid and the mature capsid shells have also been obtained [3, 4], revealing that the main protein gp10A has an HK97-like fold.

The comparison of both structures reveals the molecular basis of T7 shell maturation [4]. The mature capsid presents an expanded and thinner shell than the prohead, with a drastic rearrangement of the protein monomers that increases their interacting surfaces, in turn resulting in a new bonding lattice. The rearrangements include tilting, in-plane rotation, and radial expansion of the subunits, as well as a relative bending of the A- and P-domains of each subunit.

Our results suggest that T7 might represent one of the simplest primordial capsid maturation mechanisms.

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Single crystal X-ray diffuse scattering from supra-molecular assemblies

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Unlike Bragg scattering which only contains single body information, diffuse scattering contains two-body information and this enables the local structure and dynamics to be probed. In some instances static (occupational) disorder may feature in these studies but in others the disorder is of thermal origin and the resulting structured *thermal diffuse scattering* (TDS) is used to obtain details of the correlations that occur between both the inter- and intra-molecular displacements. Due to the recent advancements in computing power, methods that involve the construction of models of disordered crystals from which the diffuse scattering is calculated have become more and more effective.

Original methods for the evaluation of harmonic potentials used in Monte Carlo simulations for modeling the diffuse scattering from molecular crystals has been superseded by implementing an empirical formula that effectively simplifies this procedure [1]. The Method works so well that now not only is implementing disorder models (<50 atoms per molecule) more rapid (as applied to previous studies of problems associated with polymorphism in pharmaceuticals), we can also begin to accurately model the diffuse scattering features from larger supra-molecular systems. We have applied these novel techniques to problems involving supra-molecular host guest assemblies by performing simulations to model the diffuse scattering from single crystals of 1,11-undecadioic acid/urea and t-butylcalix-4-arene.

The urea inclusion compound (UIC) for 1,11-Undecadoic acid has a well resolved structure in which the guest is disordered over three positions with respect to the lattice repeat of the urea channels. A result of this disorder is strong layers of diffuse scattering perpendicular to the channel axis at one-third increments between the average 'Bragg' Layer lines. Our methods use Ising-type short-range order models for the site occupations of the guests to show that the direction for the correlation of the guest molecules between channels is actually trigonal, even though the average structure is orthorhombic. A good fit to the diffuse features is established from applying the correct correlation energies in the model.

t-Butylcalix-4-arene if crystallized with different mixtures of Pyridine-N-oxide (PNO) or Nitrobenzene ($PhNO_2$) can form what we know to be two isomorphous crystalline phases 'beta' or 'delta'. This is reflected by the apparent differences in cell dimensions and major guest occupation in the 'calix' cavity. Each of the crystals can have varying amounts of PNO or $PhNO_2$ depending on the growth