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Perspective

# Approaches Regarding the Antitoxins Generated During Immune System Responses

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## DESCRIPTION

Prokaryotes' genomes are replete with Toxin-Antitoxin (TA) systems, which form a tightly controlled network important for cell maintenance and survival under environmental challenges such antibiotic treatment, food shortage, and immune system reaction. The fact that many dangerous bacteria have several copies of the TA operon has drawn attention to this system as a potential new target for antibiotics. For instance, the bacterium that causes human disease, *Mycobacterium tuberculosis*, has approximately 80 TA systems.

Type II TA systems are the most common of the eight main types of TA systems, and they are reasonably well understood in terms of their structural makeup, biological capabilities, and feedback processes. Typically, Type II TA operons produce two short, less than 150 amino acid, and cytoplasmic proteins: a stable toxin and a rapid-turnover labile antitoxin. The toxins slow down cellular growth by impeding crucial cellular functions including protein synthesis and DNA replication. Under typical development conditions, the cognate antitoxins sterically shield the toxin active site and generate strong noncovalent contacts to oppose these effects.

A well-defined DNA-binding domain at the N-terminus, which is in charge of suppressing the cognate TA transcription, and an Intrinsically Disordered Region (IDR) at the C-terminus, which undergoes folding upon binding to the structured toxin, make up the majority of type II antitoxins. There are numerous conceivable combinations of the DNA binding domain and its nearby toxin-neutralizing IDR since DNA-binding domains are evolutionarily exchangeable between antitoxins.

There is accumulating evidence that IDRs from eukaryotes function as regulatory recognition elements, develop several layers of structure and protein-protein interaction, and have a high propensity for secondary structure. Notably, these IDRs are rich in proteins that are involved in signalling and proteins that are prone to aggregation, and they have aberrant activities or changed abundance in cells that can promote the growth of cancer or neurological diseases.

The ability of functional IDRs to adapt to stimuli and offer varied degrees of structural plasticity and heterogeneity for interactions with many partners to work is their most crucial characteristic. IDR-targeting of disease-relevant proteins in cells is a newly popular approach to medication development. Conventional biophysical approaches have had difficulty elucidating the structural specifics of the dynamics and heterogeneity of IDRs; yet, IDRs associated with diverse disorders are interesting therapeutic targets.

IDRs are less common in prokaryotes than in eukaryotes, therefore little is known about their physicochemical characteristics and functional roles in the bacterial proteome. Recent research has shown that bacterial type II antitoxins' C-terminal IDRs have conditional dynamics-based mechanisms for controlling the TA system. The functional diversity of prokaryotic IDRs has been better understood as a result of these results. Antitoxins can perform a variety of activities as a toxin binder depending on the degree of dynamics or disorder within their IDRs.

Due to the energy cost of folding, the folding-upon-binding mechanism has been thought to necessarily result in medium-to-low affinity interactions. For TA pairs, however, that have evolved to associate with a dissociation constant in the pico- to nanomolar range, this is often not the case. The advantageous intramolecular interactions of toxin-neutralizing IDRs, even in toxin-free states, as well as structural and electrostatic complementarities at the TA contact surface may be responsible for the high affinity.

These qualities might help the antitoxin get through the binding-coupled folding's high entropic cost. Additionally, conformational selection, in which only momentarily pre-existing folds within the structural ensemble are able to bind to the partner, and/or the induced fit mechanism, in which all structures within the ensemble are captured by the partner and

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subsequently fold, have both been proposed to be used in toxin neutralisation induced by antitoxin binding.

Both methods encourage IDRs to be folded or arranged in order to facilitate toxin binding. The crystal structures of TA complexes have shown that antitoxin IDRs form -helical forms that bind to the matching toxin, which is consistent with these mechanisms; however, it has been contested that the IDRs crystallise in the absence of the toxin partner. A number of type II TA systems have an inverse gene order, with the gene encoding the toxin coming before the gene encoding the antitoxins.