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Structural Identification of a Bacterial Quorum Sensing Signal Containing Boron

X. Chen, S. Schauder, I. Pelczer, B. Bassler, and F. Hughson (Princeton U.)

Beamline(s): X12C

Introduction: Cell-cell communication in bacteria is accomplished through the exchange of extracellular signaling molecules called autoinducers. This process, termed quorum sensing, allows bacterial populations to coordinate gene expression. Community cooperation likely enhances the effectiveness of processes including bioluminescence, virulence factor expression, antibiotic production and biofilm development. Unlike other autoinducers, which are specific to a particular species of bacteria, a recently discovered autoinducer (AI-2) is produced by a large number of bacterial species. AI-2 has been proposed to serve as a 'universal' signal for inter-species communication. The chemical identity of AI-2 has, however, proved elusive. Here, we present the crystal structure of an AI-2 sensor protein, LuxP, in a complex with autoinducer.

Methods and Materials: The X-ray crystal structure of recombinant *V. harveyi* LuxP was determined by multiple isomorphous replacement at 2.8 Å resolution and refined to 1.5 Å resolution using native data collected at NSLS X12C.

Results: Like other periplasmic binding proteins, LuxP consists of two similar domains connected by a three-stranded hinge. The deep cleft between the two LuxP domains contains additional electron density, corresponding to the AI-2 ligand, that was clearly visible even in initial experimental electron density maps at 2.8 Å resolution. The location of this density is clearly analogous to that of ligands in other periplasmic binding proteins. The quality of the additional electron density improved steadily as refinement of the protein model progressed until, at 1.5 Å resolution, it was straightforward to construct a model for AI-2 by positioning atoms in the difference electron density.

Conclusions: A combination of crystallographic and other evidence establishes that the bound AI-2 ligand is a furanosyl borate diester, which bears no resemblance to previously characterized autoinducers. Our findings indicate a novel biological role for boron, an element required by a number of organisms but for poorly-characterized reasons.

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