# Sequence and conformational analysis of AgrD peptides

**Implications: bacterial studies in *Staphylococcus aureus***


## *ABSTRACT*

Staphylococcus aureus is a gram positive bacterium which often colonises hosts asymptomatically, also capable of causing infections. A*ccessory gene locus (Agr)*- a two component system regulates and controls bacterial genes involved in pathogenesis.

The Agr regulatory locus consists of two divergent transcription units driven by the promoters in opposite orientation, p2 and p3. The P2 operon encodes a two-component signaling pathway consisting of four proteins, of which AgrC is the receptor and AgrA is the response regulator where as AgrB and AgrD help in secretion of an autoinducing peptide (AIP). Once the AIPs start accumulating extracellularly and reaches a threshold concentration it binds its receptor Agrc which in turn phoshorylates AgrA. Activated AgrA induces transcription from promoters P2 and P3. P3 promoter drives expression of RNAIII, the primary effector of the agr system, which was in turn activated by AgrC

Autoinducing peptides (AIPs) are 7-9 amino acid long. Based on the primary amino acid sequence of AIP's, *S.aureus* can be subdivided into 4 different *agr* groups (I, II, III, IV). Remarkably, the evolutionary *agr* locus has diverged such that the AIP's of the four different *S.aureus* groups self activate but cross-inhibit *agr* expression. However *a CYSTEINE* residue in all four peptide types is conserved across all the strains of Staphylococcus aureus which is responsible for the formation of a thiolactone ring making the AIPs functional.

This project is based on the study of sequence and conformational properties of the four different types of AIPs. A molecular dynamics study is carried out for the same.



*Key words: S.aureus, Agr, AIPs, molecular dynamics*