Oral presentation

Study of the conformational dynamics of a bacterial photoactivated adenylate cyclase

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Structural insights into the photoactivated adenylate cyclases can be used to develop new ways of controlling cellular cyclic adenosine monophosphate (cAMP) levels for optogenetic applications. OaPAC is a recently discovered blue-light using flavin adenosine dinucleotide (BLUF) photoactivated adenylate cyclase from the cyanobacterium *Oscillatoria acuminata* that uses adenosine triphosphate and translates the light signal into the production of cyclic adenosine monophosphate [1,2]. Here, we report the crystal structures of the enzyme in the absence of its natural substrate determined from room temperature serial crystallography data collected at both an X-ray free electron laser and a synchrotron and we compare them with the cryo macromolecular crystallography structures obtained at a synchrotron by us [3] and others [1,2,4]. These results reveal slight differences in the structure of the enzyme due to data collection at different temperatures and X-ray sources. We further investigate the effect of the Y6 mutation in the blue-light using flavin adenosine dinucleotide domain, a mutation which results in a rearrangement of the hydrogen-bond network around the flavin and a notable rotation of the side-chain of the critical Q48 residue [3]. These changes in the hydrogen bond network around the flavin triggered by the mutation point towards an allosteric regulation mechanism for the enzyme and are discussed in the light of the small and large-scale movements observed in the enzyme in solution upon ATP binding [5].

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