

**A METHOD FOR INVESTIGATING THE PROPAGATION OF
MOTIONS OF REMOTE SURFACE RESIDUES INTO THE BURIED
CATALYTIC SITE OF RUBISCO BY MOLECULAR DYNAMICS**

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Rubisco (ribulose-1,5-bisphosphate carboxylase/oxygenase) is the crucial and rate limiting enzyme in the biomass producing pathway of photoautotrophic organisms. It catalyzes two competing reactions: the fixation of inorganic carbon to a C₅ compound (ribulose-1,5-bisphosphate) as well as the oxygenation of this substrate, whereas the latter reaction initiates the energy consuming respiratory pathway. Key figures for comparing different Rubisco species are their specificity towards carboxylation and the turnover of this reaction.

Laboratory experiments show that *in vitro* mutagenesis of residues distant from the buried binding site (which in closed, loaded state is sealed by several structural elements like the C-terminal tail and loop 6) may have a high impact on the aforementioned performance criteria of the enzyme [1].

The "time-window" hypothesis explains the implication of repeated perturbations of the catalytic process after ligand binding on the specificity of a given Rubisco species [2]. These interruptions may be exerted by fluctuations of important residues in the catalytic site or larger conformational changes like a partial opening of the binding pocket.

By covariance and correlation analyses of highly sampled molecular dynamics trajectories the concerted motions of atoms can be investigated and quantified [3]. Methods for enhancing the significant information from the bulk of data gained have been developed and applied to simulation results of wild type and *in silico* mutant Rubisco structures of *Synechococcus*.

This approach may aid us to identify yet unknown important residues remote from the binding niche and to reveal the mechanism of intramolecular propagation of dynamics relevant to catalysis.

REFERENCES

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