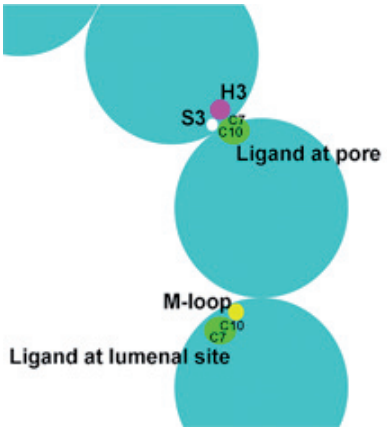
docking techniques and molecular dynamics simulations. Modeling results indicate that positions C7 and C10 affect the conformation of three key elements (the M-loop, S3 and H3) in the lateral interactions that modulate the contacts between adjacent protofilaments. Alternatively, the change in C2 slightly rearranges the ligand in the binding site, thus modifying the interaction of the ligand C7 position with the M-loop.



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Scheme of the interactions of taxane ligands at the pore and luminal binding sites of microtubules, with the structural elements responsible for the interprotofilament interaction. The microtubule protofilaments are seen from the plus end

Key words: SAXS, protein, assembly, NMR, molecular dynamics

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A redox-controlled synergistic mechanism regulates the binding of the intrinsically disordered protein CP12 to photosynthetic glyceraldehyde-3-phosphate dehydrogenase

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Carbon assimilation in plants is regulated by the reduction of specific protein disulfide bridges by light and their re-oxidation in the dark [1]. The redox switch, CP12, is a small, intrinsically-disordered protein that carries two disulfides groups. In the dark, it forms an inactive supramolecular complex with glyceraldehyde-3-phosphate dehydrogenase (GAPDH) [2],[3]. Here we show that binding of CP12 to GAPDH follows a synergistic mechanism that includes both conformational selection and induced folding steps. Initially, a conformation characterized by a circular structural motif of the C-terminal disulfide of CP12 is selected by GAPDH. Subsequently, the induced folding of the flexible C-terminal tail of CP12 in the active site of GAPDH site stabilizes the binary complex. Formation of several hydrogen bonds compensates the entropic cost of CP12 fixation and terminates the synergistic mechanism that controls carbon assimilation.

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Keywords: photosynthesis, enzyme, complex

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Rotor architecture in the yeast F_1-c_{10}-ring complex of F-ATP synthase

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F_1F_o-ATP synthase is a hybrid molecular nanomotor. F_1 is a chemical motor driven by ATP hydrolysis while F_o is an electrical motor driven by the proton flow. The two stepping motors are mechanically coupled through a common rotary shaft. The F_1-ATPase X-ray structures support binding change mechanism for catalysis. The empty and open catalytic site β_E is the OPEN site with low affinity for nucleotides, the β_{TP} site filled by ATP (or AMP-PNP) is the LOOSE conformation and the β_{DP} site filled by ADP is the TIGHT conformation where synthesis occurs. In F_1 domain, the orientation of the γ-subunit relative to the $(\alpha\beta)_3$ component determines the catalytic state of the enzyme and, according to the binding change mechanism, a 120° rotation of the γ-subunit during the ATP hydrolysis cycle results in E→TP, TP→DP and DP→E interconversions.

Up to now, the three available crystal structures of the F_1c_{10} sub-complex of the yeast F_1F_o-ATP synthase were isomorphous [1] and [2] with a crystal form named yF_1c_{10}(I).

In the crystal structure of the Mg.ADP-inhibited state of the yeast F_1c_{10}-ATP synthase, solved at 3.4 Å resolution, an ADP molecule was bound in both β_{DP} and β_{TP} catalytic sites [1]. The α_{DP}-β_{DP} pair is slightly open and resembles the novel conformation identified in the yeast F_1 [3], whereas the α_{TP}-β_{TP} pair is very closed and resembles more a DP pair. In the F_o rotor ring, the essential cGlu59 carboxylate group is only surrounded by apolar residues. Its closest hydrogen bond acceptor, the cLeu57 carbonyl oxygen of the adjacent c-subunit, is too far away to make a direct hydrogen bond. The proton binding has specific features compared to the bacterial Na^+-transporting or the cyanobacterial and chloroplastic H^+-transporting F-type ATP synthase rotor structures. In the crystal, significant interactions of the c_{10}-ring with the F_1-head of neighboring molecules affect the overall conformation of the F_1-*c*-ring complex. The symmetry axis of the F_1-stator and the inertia axis of the *c*-ring are tilted near the F_1-F_o rotor interface, resulting in an unbalanced machine.

Recently, we have solved a new crystal form of the yeast *Saccharomyces cerevisiae* F_1c_{10} complex, named yF_1c_{10}(II), inhibited by adenylyl imidodiphosphate (AMP-PNP) and dicyclohexylcarbodiimide (DCCD), at 6.5 Å resolution in which the crystal packing has a weaker influence over the conformation of the F_1-*c*-ring complex.

Despite a low resolution, the overall fold is clearly visible with a more straight C-terminal helix of subunit γ. Though the F_1-stator is 8° tilted relative to the rotor axis, its center of mass is located approximately on this axis. Therefore, yF_1c_{10}(II) provides a model of a more efficient generator. The present yeast yF_1c_{10}(II) and the bovine bF_1c_8 [4] models are comparable and together provide accurate models of the F_1-*c*-ring domain in the intact F_1F_o-ATP synthase.

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