crystal structure of human T-protein with folate cofactor and provided the insight into the molecular basis of the disease-causing mutations. Here we present the crystal structure of *Escherichia coli* T-protein in complex with dihydrolipoate-bearing H-protein and 5-methyltetrahydrofolate (5-CH_3-THF): a complex mimicking the ternary complex in the reverse reaction. The structure of the complex shows a highly interacting intermolecular interface limited to a small area and the protein-bound dihydrolipoyllysine arm inserted into the active site cavity of the T-protein. Among the residues contributing to the interface, invariant Arg292 of the T-protein plays a key role in the complex assembly and probably in recruiting the aminomethyllipoyllysine arm to the active site of T-protein. It has been speculated that the aminomethyltransfer reaction from aminomethyllipoate of H-intermediate to THF is initiated by the direct attack of the methylene carbon atom by the nucleophilic N5 or N10 atoms of THF bound to T-protein accompanying the release of ammonia. However, the distances between the tip of the dihydrolipoyllysine arm and the methyl carbon atom of 5-CH_3-THF observed in the complex structure suggests the presence of an intermediary mediating the transfer reaction rather than the direct interaction. The hydrogen bond network surrounding the S8 atom of the dihydrolipoyllysine including invariant Asp96, Asp97, Asn113, and Arg223 of T-protein suggests that the reversible transfer of the methylene group between the lipoate and tetrahydrofolate should proceed through the electron relay-assisted iminium intermediate formation. Based on the structural observations together with mutational analyses, we propose a possible mechanism for T-protein catalysis. The structure also provides novel insights in understanding the disease-causing mutations, in addition to the disease-related impairment in the cofactor-enzyme interactions presented previously.

Keywords: Protein_complex, Catalytic_reaction

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Molybdenum Oxide/Bipyridine hybrid materials: synthesis, structure and catalytic studies

Tatiana R. Amarante,[a] Marta Abrantes,[b] Margarida M. Antunes,[a] Sandra Gago,[a] Filipe A. Almeida Paz,[a] Martyn Pillinger,[a] Anabela A. Valente,[a] Isabel S. Gonçalves.[a] [a]*Departament of Chemistry, CICECO, University of Aveiro, 3810-193 Aveiro, (Portugal).* [b]*Centro de Química Estrutural, Complexo Interdisciplinar, Instituto Superior Técnico, Universidade Ténica de Lisboa, Av. Rovisco Pais, 1, 1049-001 Lisboa, (Portugal).* E-mail: tatiana.amarante@ua.pt

The chemistry of Mo(VI) is very important in industrial and biological systems [1, 2]. Monomeric complexes of the type $[MoO_2X_mL_n]$ (X = mono/dianionic ligand, L = neutral ligand) have been shown to be active catalysts, or catalyst precursors, for homogeneous epoxidation of non-functionalized olefins. Recently we found that $[MoO_2Cl_2(bipy)]$ (bipy = 2,2'-bipyridine) can produce a molybdenum(VI) oxide-based hybrid material [3] which can be used as an heterogeneous catalyst.

The molybdenum oxide/bipyridine hybrid material $\{[MoO_3(bipy)][MoO_3(H_2O)]\}_n$ can be isolated as a microcrystalline powder, in yields of 72-92%, from the reaction of $[MoO_2Cl_2(bipy)]$ in water using three distinct methods: hydrothermal (100ºC, 19h), reflux (120ºC, 4h) and microwave (120ºC, 4h).

The crystal structure of this hybrid material was determined from synchrotron X-ray powder diffraction data. The material is composed of two distinct neutral one-dimensional polymers: an organic-inorganic polymer, $[MoO_3(bipy)]_n$, and a purely inorganic chain, $[MoO_3(H_2O)]_n$; the two are interconnected by O-H···O hydrogen bonding interactions.

The material is a moderately active, stable, and selective catalyst for the epoxidation of *cis*-cyclooctene at 55 ºC with *tert*-butylhydroperoxide (*t*BuOOH, 5.5 M in decane or 70% aqueous) as the oxidant. Within the process, biphasic solid-liquid or triphasic solid-organic-aqueous mixtures are formed, and 1,2-epoxycyclooctane is the only reaction product. When *n*-hexane is employed as a co-solvent and *t*BuOOH(decane) is the oxidant, the catalytic reaction is heterogeneous in nature, and the solid catalyst can be recycled and reused without loss of activity. For comparison, the catalytic performance of the precursor $[MoO_2Cl_2(bipy)]$ was also investigated. The FT-IR spectra of the solids recovered after catalysis indicate that the discrete complex transforms into the organic-inorganic polymer $[MoO_3(bipy)]$ [4] when the oxidant is *t*BuOOH(decane) and compound $\{[MoO_3(bipy)][MoO_3(H_2O)]\}_n$ when the oxidant is 70% aqueous *t*BuOOH.

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Structural and functional analysis of rRNA methyltransferase from *Staphylococcus aureus*

Shunsuke Kita,[a] Yoshikazu Tanaka,[a,b] Min Yao,[a,c] Isao Tanaka,[a,c] [a]*Graduate School of Life Science, Hokkaido University.* [b]*CRIS, Hokkaido University.* [c]*Faculty of Advanced Life Science, Hokkaido University, Sapporo (Japan).* E-mail: kita@castor.sci.hokudai.ac.jp

Ribosomal RNAs (rRNAs) are modified post-transcriptionally to generate variety of nucleotides required for fine tuning of ribosomes. In *Escherichia coli*, m2G 2445 of 23S rRNA is produced by *Ec*RlmL (ribosomal large subunit methyltransferase L), which possesses two methyltransferase domains. In *Staphylococcus aureus*, these two domains are separated two proteins, *Sa*RlmL-N and *Sa*RlmL-C. Here we present crystal structure and RNA binding study of *Sa*RlmL-N and *Sa*RlmL-C.

SaRlmL-N and *Sa*RlmL-C were expressed in *E.coli* and purified by Ni-affinity chromatography and size exclusion chromatography. Crystals were obtained by using vapor diffusion method and X-ray diffraction data were collected at BL41XU SPring-8, Harima, Japan and PF BL-17A, Tukuba, Japan. crystals of *Sa*RlmL-N *Sa*RlmL-C belong to space group $P2_1$ with cell dimensions (*Sa*RlmL-N: a = 52.5, b = 107, c = 77.2 Å, β = 100° ; *Sa*RlmL-C: a = 95.8, b = 91.7, c = 103 ∓, β = 93.9−). structures were solved by molecular replacement with the program *Morlep*.

Structure of *Sa*RlmL-N contains methyl donor, *S*-adenosyl-methionine (SAM) in methyltransferase domain. SAM binding pocket is connected to vast cleft which is charged positive and surrounding residues are highly conserved. RNA binding experiments were performed using *in vitro* transcribed RNA fragment including Guanine 2445. Formation of *Sa*RlmL-N and RNA fragment complex was confirmed by size exclusion chromatography. This result indicates that *Sa*RlmL-N may serve as m2G 2445 methyltransferase in *S. aureus*. ased on the structur and RNA binding study, we propose the RNA binding model of *Sa*RlmL-N.

Structure of *Sa*RlmL-C is composed three domains: NTD, EEHEE and MTase, and is similar to *Ec*RlmI with different intermolecular