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Crystal Structure of the CcbJ Methyltransferase from *Streptomyces caelestis* [1]

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CcbJ is an S-Adenosylmethionine (SAM) dependent methyltransferase from *S. caelestis* which catalyzes the final step in the biosynthesis of the antibiotic celesticetin. *S. caelestis* has exhibited the ability to synthesize different derivatives of celesticetin depending on the presence of different salicylic acid derivatives in the growth medium. [2] In order to understand how this organism is able to manage this, we have isolated, overexpressed, and purified the individual components of this pathway, including CcbJ [3].

The crystal structure of free CcbJ was determined by Multiwavelength Anomalous Dispersion and that of the CcbJ–SAM complex was determined by molecular replacement (using the free structure as the search model). In both structures CcbJ crystallized in the C22₁ space group with unit cell lengths of $a = 168.02$, $b = 244.55$, and $c = 117.85$. In both crystals, the asymmetric unit contained six monomers arranged as a dimer of trimers.

CcbJ possesses the class I SAM-dependent methyltransferase fold [4], [5]; modifications to the core fold include insertion of a four-stranded β -sheet, which serves as an active site cover, between αE and $\beta 5$ and a short 3_{10} helix between $\beta 4$ and αD , which forms part of the SAM binding cleft. There is also an extension to the N-terminus. These insertions match the general pattern seen in other small-molecule methyltransferases. Overall, CcbJ appears to be most similar to glycine N-methyltransferase (GNMT) which also has a similar active site cover and a 3_{10} helix in the SAM binding cleft. Aside from a similar overall shape, the active site of CcbJ is quite different from that of GNMT, having a much larger number of aromatic residues.

One of the most characteristic features of CcbJ is the great degree of flexibility exhibited by the residues in the N-terminal extension preceding αZ . In the free CcbJ structure, these residues were completely disordered in one of the six chains and none of the residues preceding Tyr-17 were visible. In the CcbJ–SAM complex, however, the entire extension was visible in all six chains. The newly ordered residues form an α -helix which passes between the active site cover and αB and forms part of the SAM binding site. Following this helix, the extension passes over part of the active site opening before entering helix αZ . The loop between these two helices contains several proline and glycine residues and is likely to be natively unstructured. This would probably allow it to adopt several different conformations which might allow it to accommodate the several different substrates observed *in vivo* [2].

[1] This research was supported by VEGA 2/0122/11 in Slovakia and MŠMT 2B08064 in the Czech Republic. [2] A.D. Argoudelis, J.H. Coats, L.E. Johnson, *J Antibiotics* **1974**, 27, 738–743. [3] L. Čermák, J. Novotná, Ságová-Marečková, M. Kopecký, J. Najmanová, L. Janata, J. Folia Microbiol **2007**, 52, 457–462. [4] J.L. Martin, F.M. McMillan, *Curr Opin Struct Biol* **2002**, 12, 783–793. [5] H.L. Schubert, R.M. Blumenthal, X. Cheng, *TRENDS Biochem Sci* **2003**, 28, 329–335.

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1 and 2-D metal-organic polymer of Sc(III) with sulfonate-carboxylate ligand

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Reaction of scandium chloride with 3,5- disulfobenzoic acid[1] under hydrothermal conditions leads to the formation of two metal-organic polymer compounds [$\text{Sc}_2(\text{3,5-DSB})_2(\text{HO})_3(\text{H}_2\text{O})_2$] (**1**) and [$\text{Sc}_2(\text{3,5-DSB})_2(\text{HO})_2(\text{H}_2\text{O})_2$] (**2**) that crystallize in the triclinic space group P-1. In both cases, the oxygen atoms of the carboxylate group are linking two metallic centers in $\mu_1 \mu_1 \eta^2$ mode. Two hydroxyl groups act as bridges linking scandium (III) cations along [011] direction. In the axial positions the scandium is coordinated by the oxygen of the sulfonate group, which is in *anti* coordination $\mu_1 \eta^1$ mode. Two water molecules are coordinated in equatorial and axial positions. This arrangement allows the formation of bidimensional polymeric structure arranged in layers along (100) plane. The difference between the compounds **1** and **2** is the substitution in the compound **2** of one bridge hydroxyl molecule by one oxygen atom of the sulfonate group ($\mu^1 \mu^1 \eta^2$) along the [011] direction.

The utilization of a auxiliary ligand 1,10-Phenanthroline[2], under conditions similar to previous leads to formation of [$\text{Sc}(\text{3,5-DSB})(\text{Phen})(\text{H}_2\text{O})_2(\text{H}_2\text{O})$]. In this compound the Sc(III) is hepta-coordinated by the phenanthroline chelate, one water molecule and a carboxylate group in $\mu_1 \mu_1 \eta^1$ mode in equatorial position and with two sulfonate groups (*anti* $\mu^1 \eta^1$ mode) in axial position. The *trans* disposition of the ligand allows the formation of polymeric chains that grow along the *c* axis in “ladder” form. The chains are linked by hydrogen bonds along *b* direction; π - π slipped stacking interactions between the rings of the phenanthroline give rise to 3D supramolecular structure.

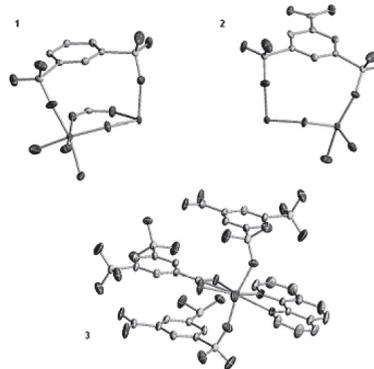


Fig 1. ORTEP drawing of the asymmetric units for **1-3** compounds; ellipsoids are displayed at the 50% probability level.