# The first crystal structure of a family 31 carbohydrate-binding module with affinity to beta-1,3-xylan.

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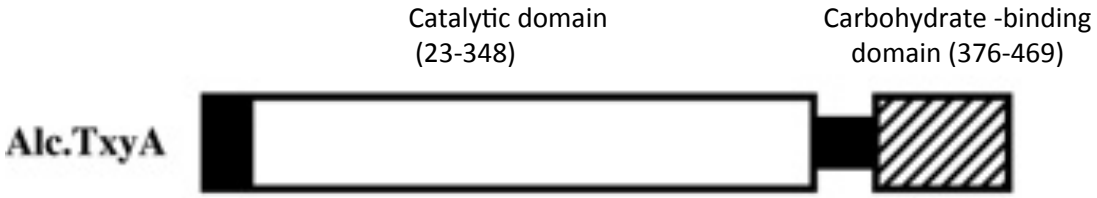
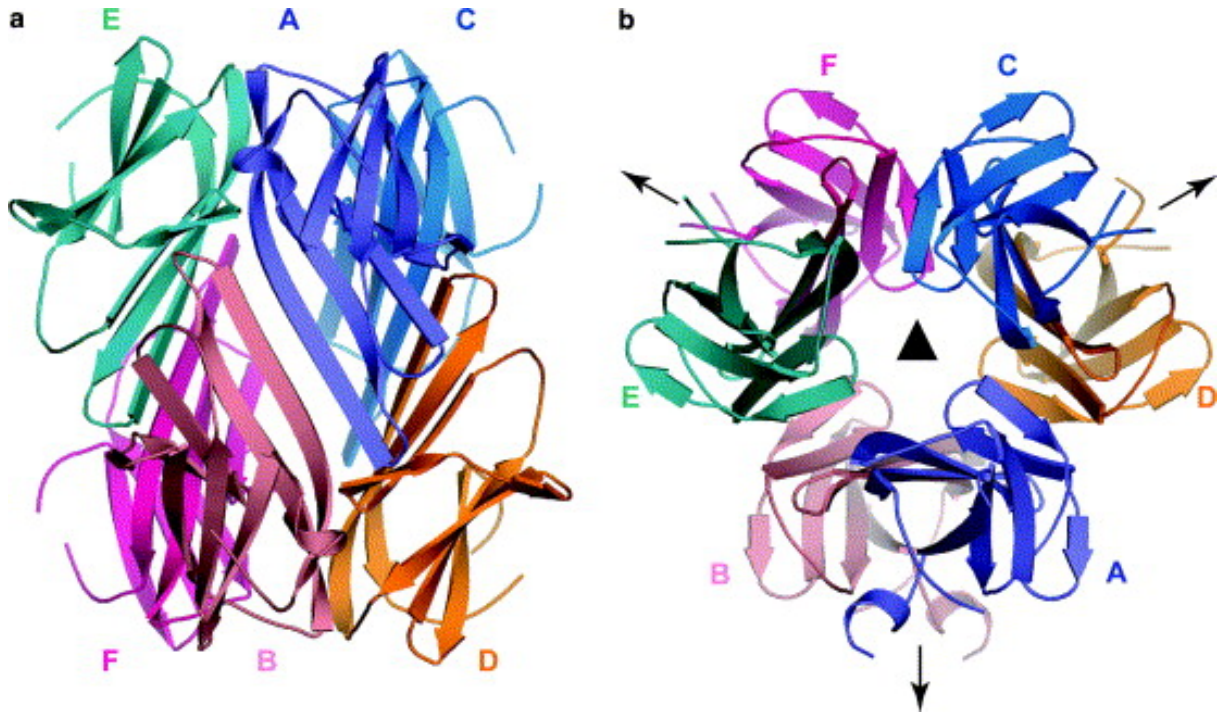
# *Alc*CBM31

- CBM of β-1,3-xylanase from *Alcaligenes* sp. strain XY-234 (Txy-A)
- Xylanase is a glycoside hydrolase; a modular protein composed of catalytic modules and a non-catalytic carbohydrate-binding module (CBM)




- The CBD has a hexameric structure.

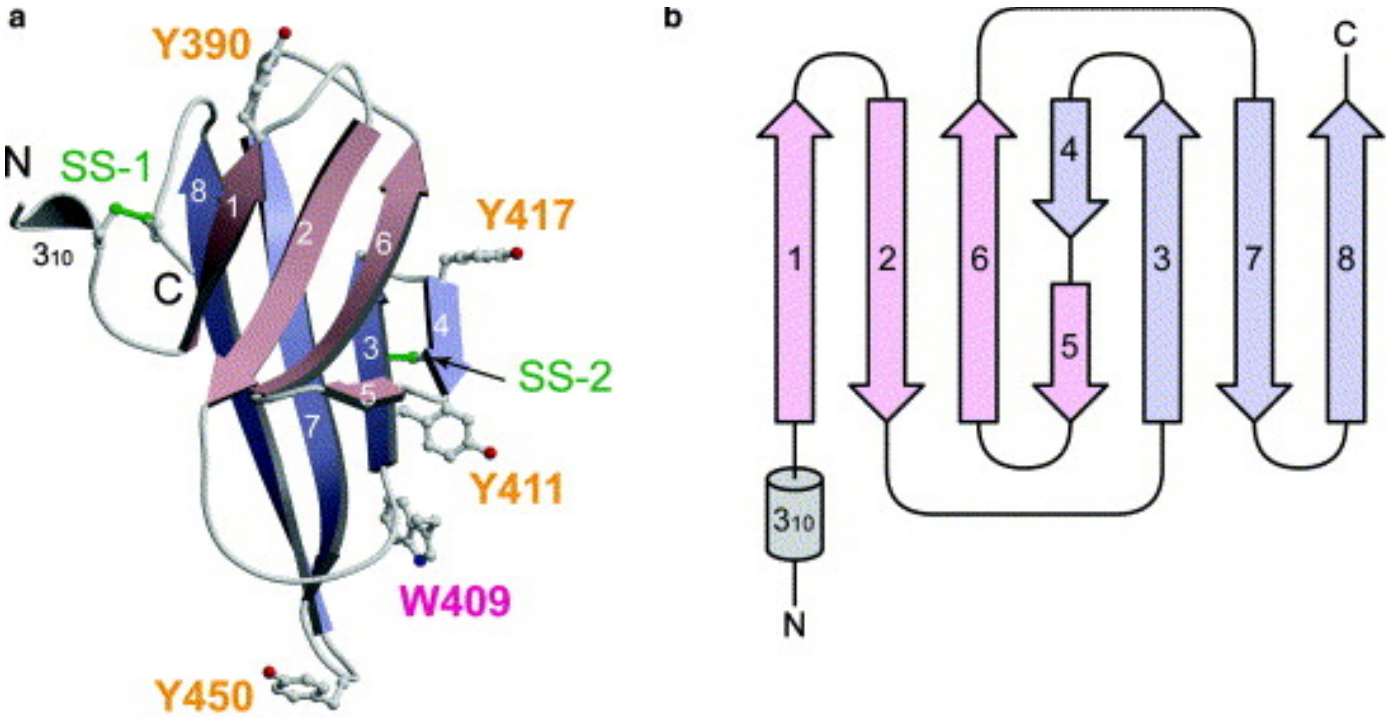
# Overall structure of *Alc*CBM31




a) Hexameric structure of *Alc*CBM31 in the asymmetric unit.;
Six molecules A,B,C,D,E, F form a spherical hexamer.
The hexamer is a trimer of dimers; AB, CD, EF; in each dimer β8 interacts with the other monomer in anti-parallel manner. This forms a large eight-stranded antiparallel β-sheet between 2 monomers.

b) Top view of Non-crystallographic symmetries are shown. A black triangle and three black arrows indicate pseudo 3-fold and pseudo 2-fold symmetries, respectively.

# Monomeric *Alc*CBM31

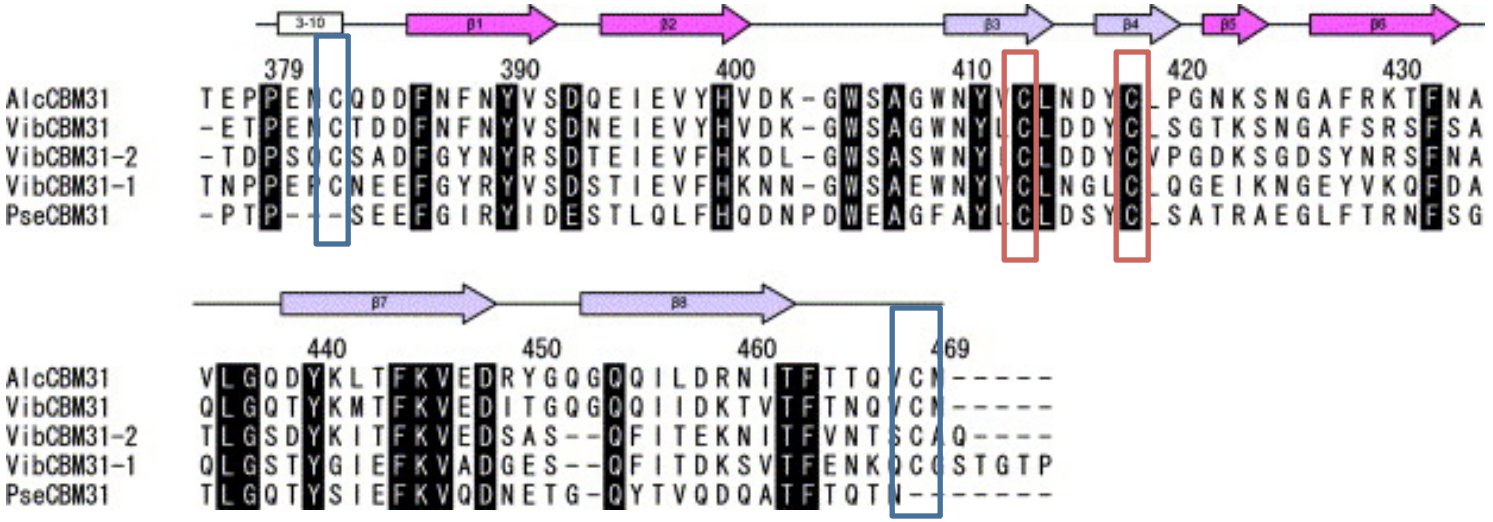



- Monomeric *Alc*CBM31 which consists of **8 β-strands (β1- β8), and one helix ($3_{10}$).**
- Forms an immunoglobulin fold; β1, β2, β6, β5 in one anti-parallel sheet, and facing β4, β3, β7, β8 in another anti-parallel sheet.
- Two intra-molecular **disulfide bonds** (SS-1 and SS-2):

  Cys382 and Cys468: SS-1 between C- and N-terminus, and stabilize the loop regions.

  Cys413 and Cys417: SS-2 between β3 and β4.

# Sequence alignment of five CBM31s




- *Alc*CBM31, *Vib*CBM31, *Vib*CBM31-1, *Vib*CBM31-2 and *Pse*CBM31
- Cys413, and Cys417 that form SS-2 are conserved in all CBM31s.→ structure-function relationship.
- Cys382 and Cys 468 that form SS-1 are conserved in 4 → structural stablization