SPECTRAL ANALYSIS AND STRUCTURAL MODELING OF CYTOCHROME B561 PROTEINS

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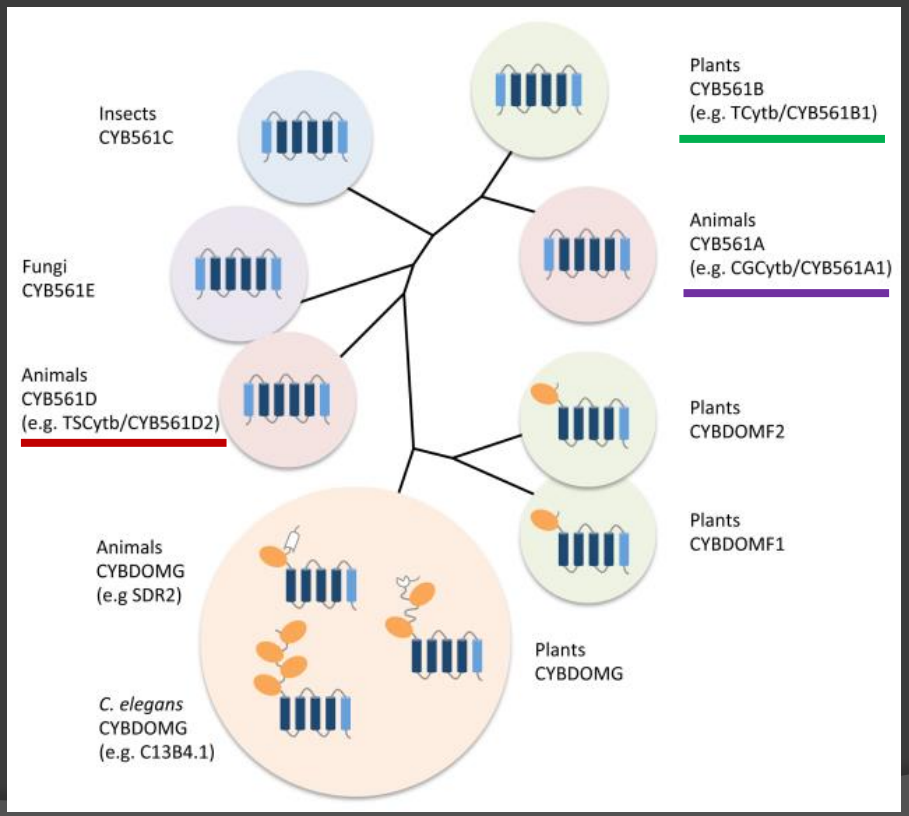
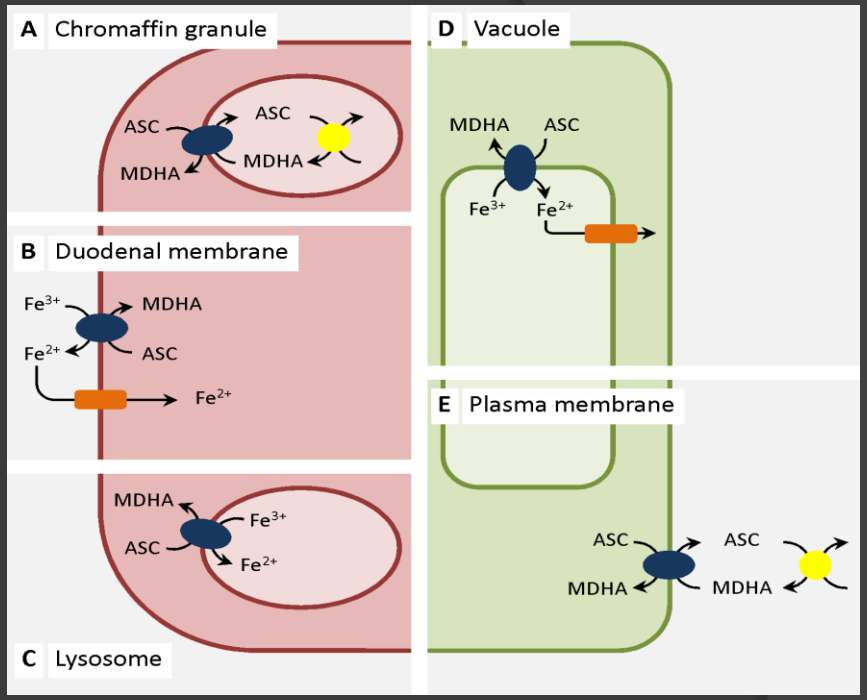
The cytochrome *b*561 protein family: 6 transmembrane alfa helix proteins with 2 b-type hemes on each side of the membrane.

Function: electron transport across the membrane from cytoplasmic ascorbate to various electron acceptors.



Asard et al. (**2013**) *A&RS* **19:** 1026-1035.



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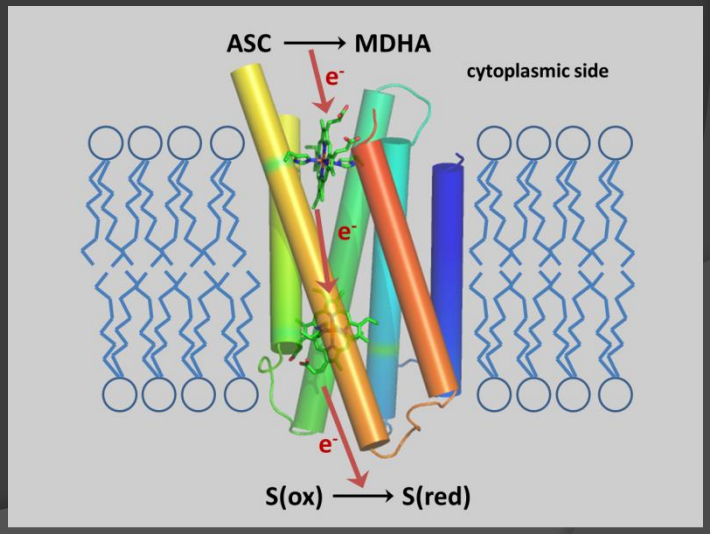
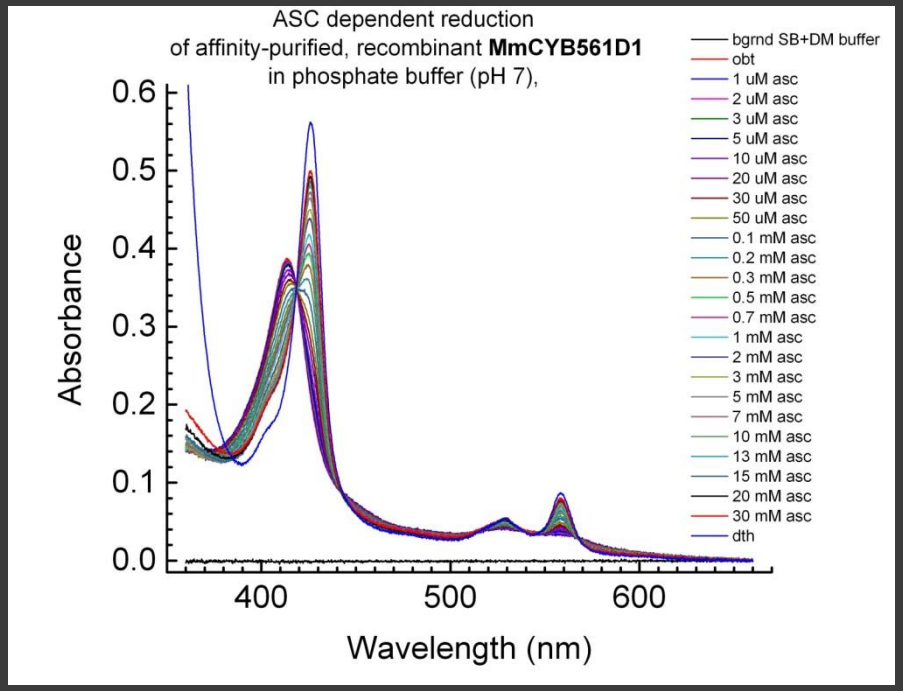
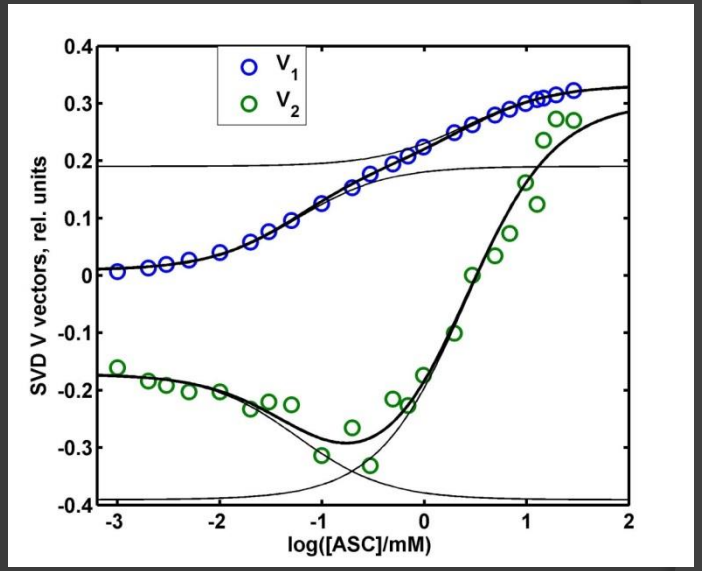
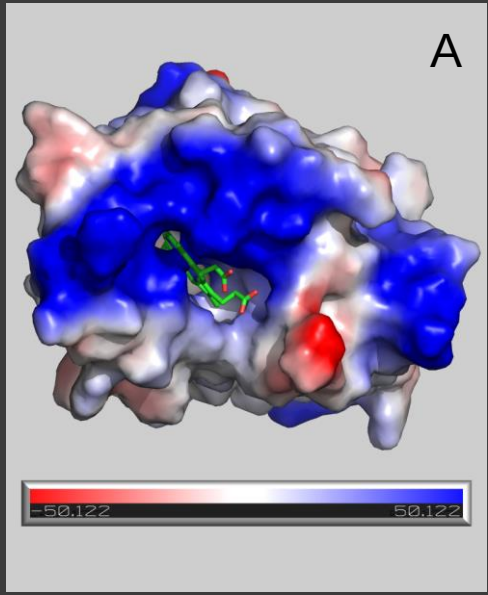


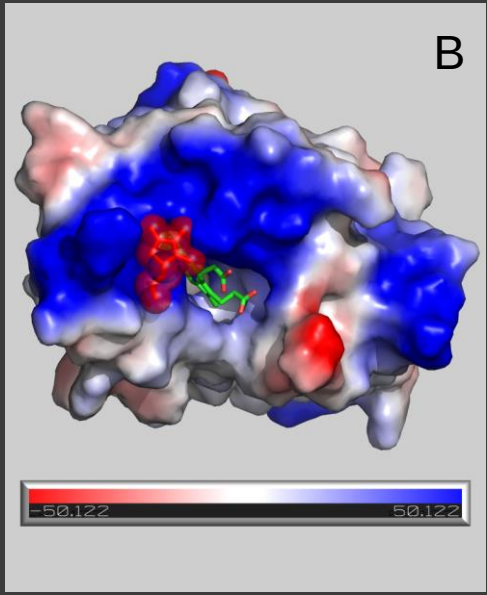
Based on the crystal structure of AtCYB561B2; 4O6Y.pdb, Lu et al. PNAS 111 (2014) 1813

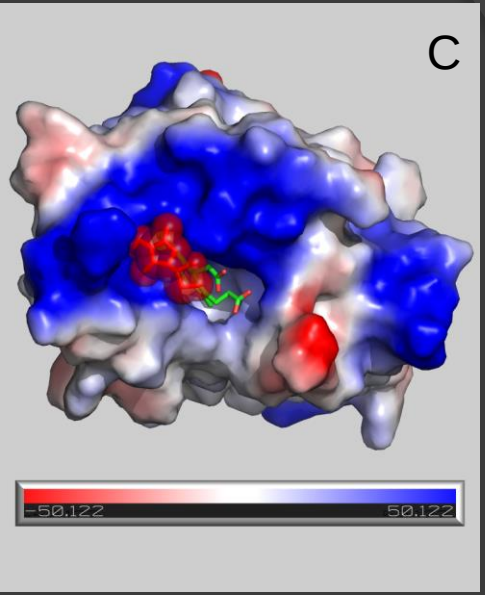
Ascorbate titration of the novel, mouse Cytb561 D1 protein.
Singular Value Decomposition of the spectra reveal 2 slightly different spectral forms, and fit of the V vectors yields 2 apparent binding constants for ASC. This is typical for all Cytb561 studied so far.

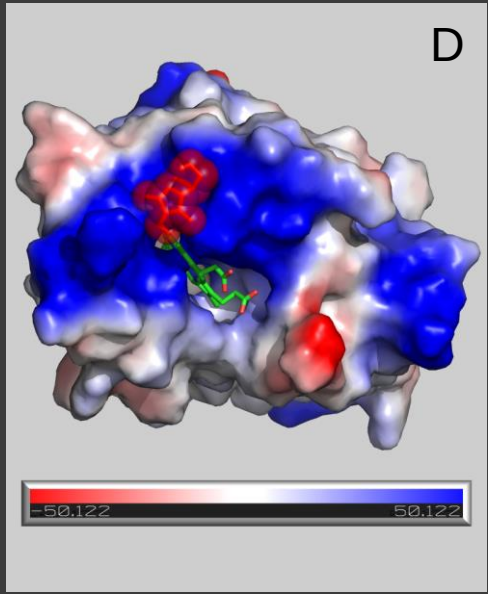


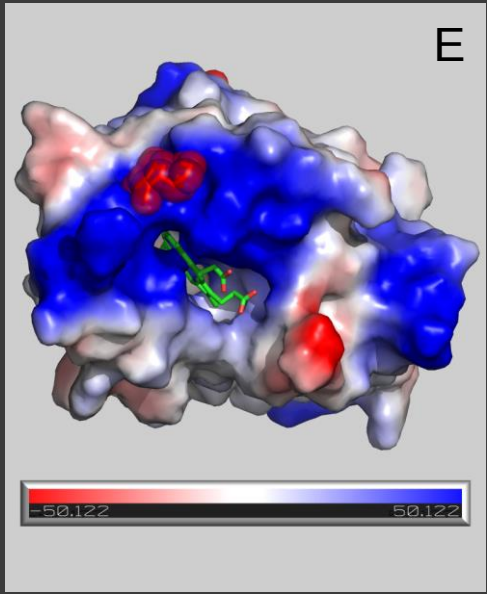


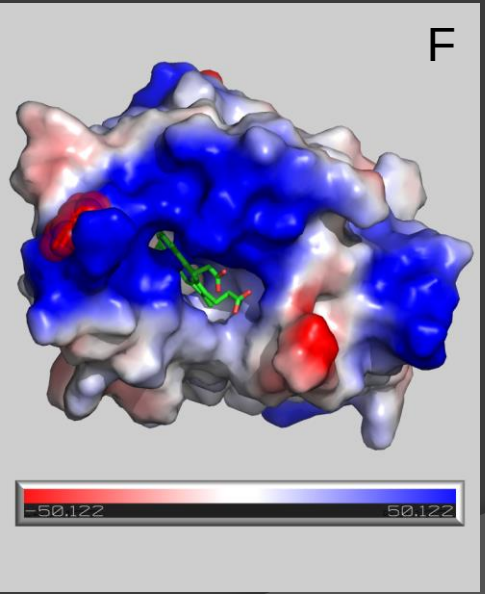












A:
crystal
structure

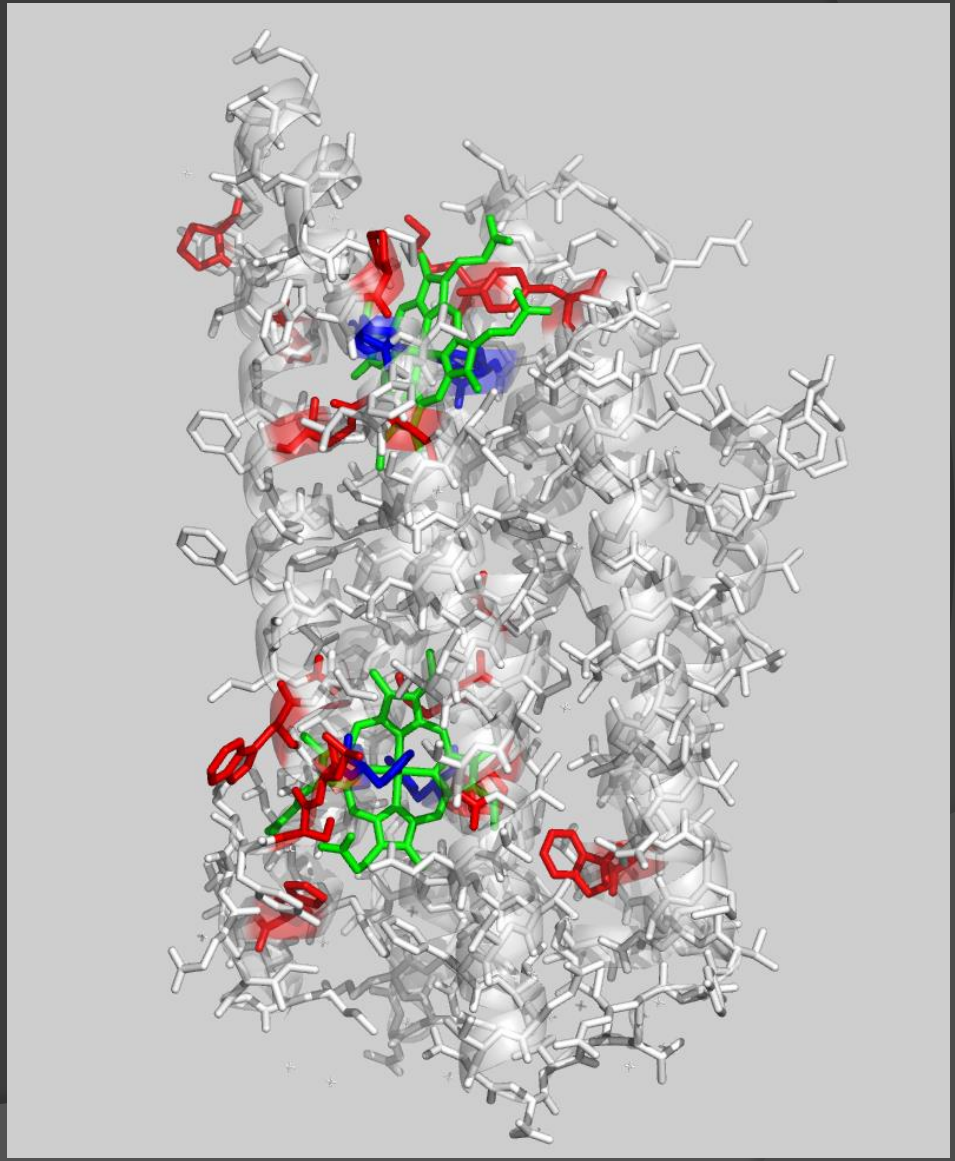
B:
crystal
structure with
bound ASC

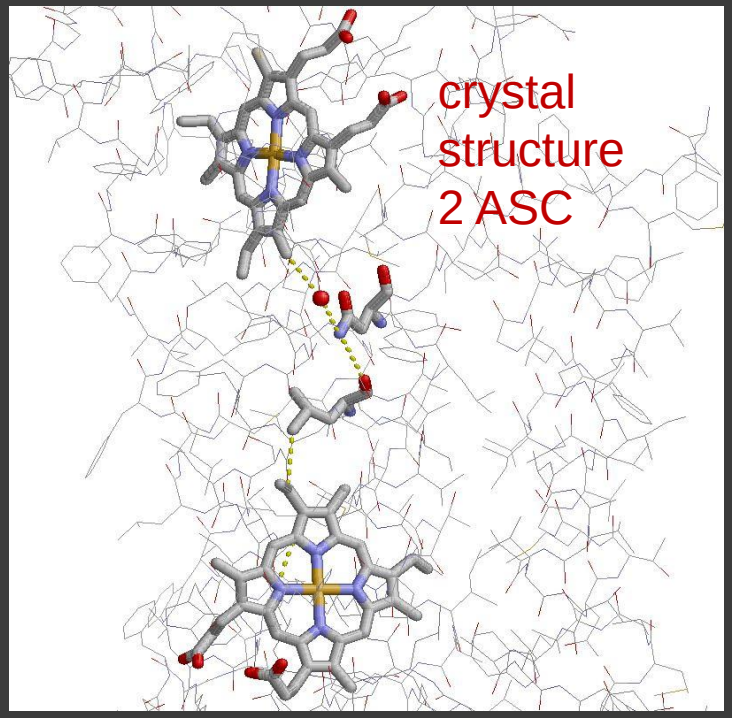
C-F:
calculated
docking
poses of ASC

More than 2, almost equally strong docking sites found *in silico*. But! A model taking into account the gradually decreasing solution redox potential with increasinc [ASC] also reproduces the two-phase reduction of Cytb561, without assuming docking sites.

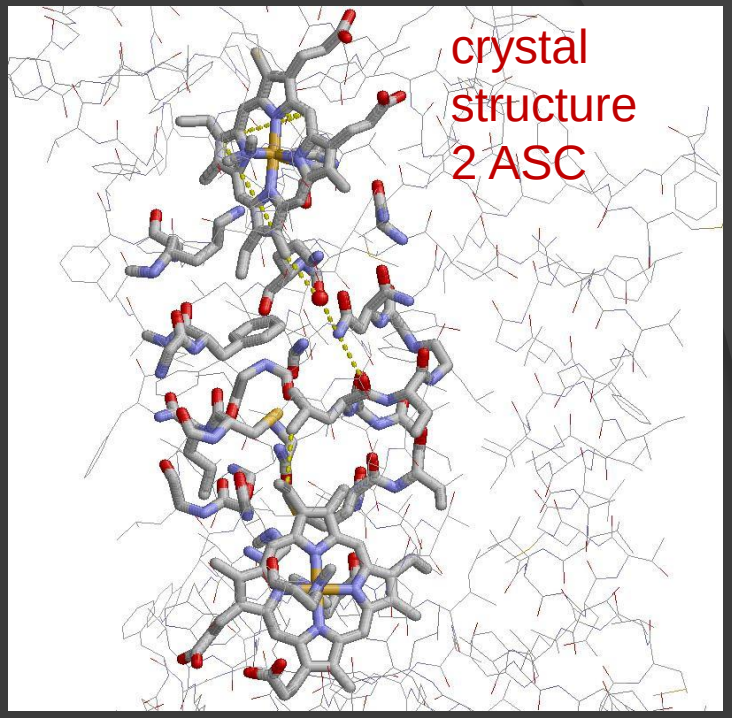
Structure of the crystallized Cytb561. Homology modeling of 10 further family members yielded very similar structures. Green: hemes, blue: fully conserved axial His ligands, red: fully and strongly conserved amino acids.

There are no conserved amino acids between the two hemes!





Best electron transfer pathway.



Atoms involved in further electron transfer pathways with not less than 10% of the efficiency of the best pathway.

The packing density model of intraprotein electron transfer mechanism seems adequate for the transmembrane electron transfer in Cytb561 proteins. No specific pathway is conserved between the two hemes.