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Fingerprint and Structural Analyses in a Putative Short Chain Oxidoreductase Enzyme. Robert Huether¹, Bi-Cheng Wang⁴, James Zhi-Jie Liv⁴, Vladimir Pletnev³, Timothy Umland¹², Qilong Mao², Leah Gambino², and William Duax¹, ¹SUNY at Buffalo Dept of Structural Biology, NY 14203 ²Hauptman-Woodward MRI NY, 14203, ³Inst. Bioorg. Chem., RAS, Moscow Russia ⁴Univ. of Georgia, Georgia, 30602.

We have identified a highly conserved fingerprint of 40 residues in the TGxxxGIG subfamily of the Short chain oxidoreductase (SCOR) enzymes. The subfamily is made up of over 7900 members with an amino acid length of ~250. The 40 fingerprint residues are critical to catalysis, cofactor binding, protein folding and oligomerization. They give us insight into evolution of the folding and function of SCORs enzymes. We have identified a putative SCOR enzyme from *C. thermocellum* (Cth1068) that contains 30 of the 40 fingerprint residues. Of the 10 variants from the fingerprint, one is a Gly substitution of a highly conserved Asn residue that plays significant structural and catalytic roles; no previously reported TGxxxGIG SCOR crystal structure contains this N→G mutation. We are undertaking crystal structure analysis to determine the impact of this variation on the hydride transfer network, the conformation of helix 5 and oligomer formation. We have a 1.8Å resolution dataset on a tetragonal crystal form (I4₁22). Supported by NIH Grant No. DK26546 (WLD)