

Mechanistic and Structural Analyses of the Roles of Arg409 and Asp402 in the Reaction of the Flavoprotein Nitroalkane Oxidase^{†,‡}

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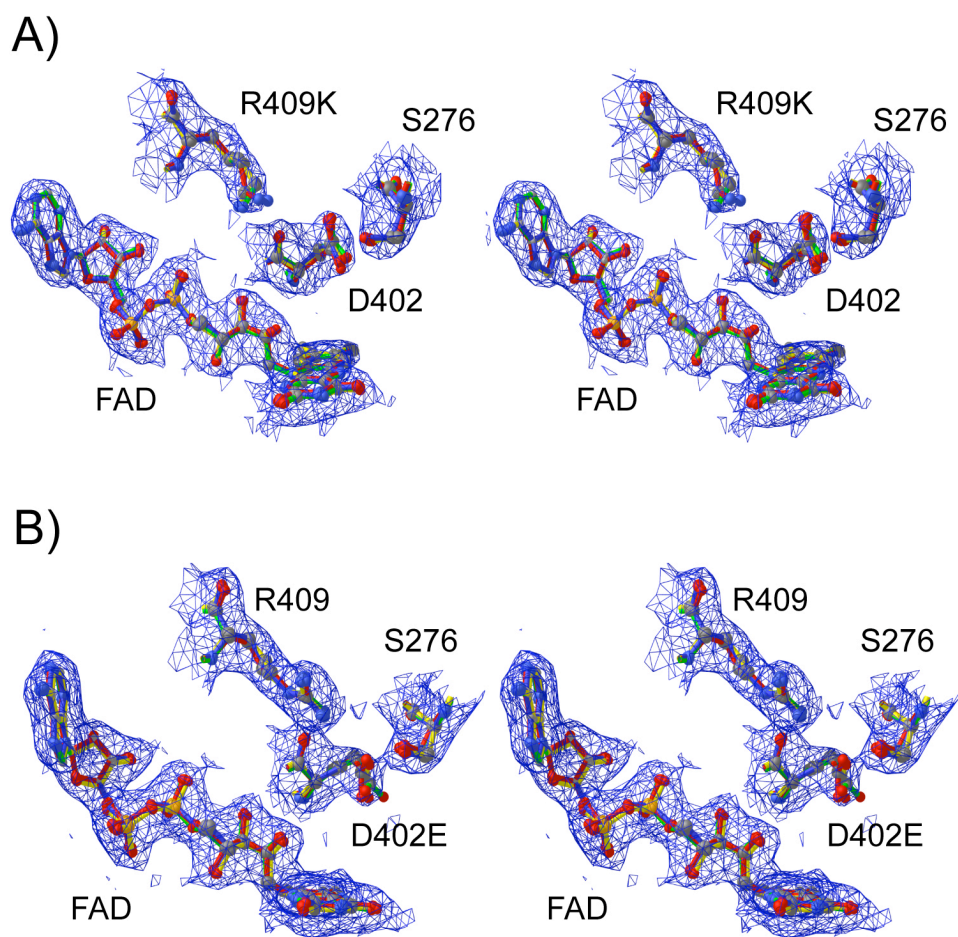


Fig. S1: Divergent stereo views of the NCS averaged electron density maps (1 σ) for (A) R409K and (B) D402E at 2.65 Å and 2.4 Å resolution, respectively. All four subunits are superimposed within the density with bonds shown in yellow, blue, green and red for subunits A,B,C,and D, respectively. Atoms are colored according to atom type.

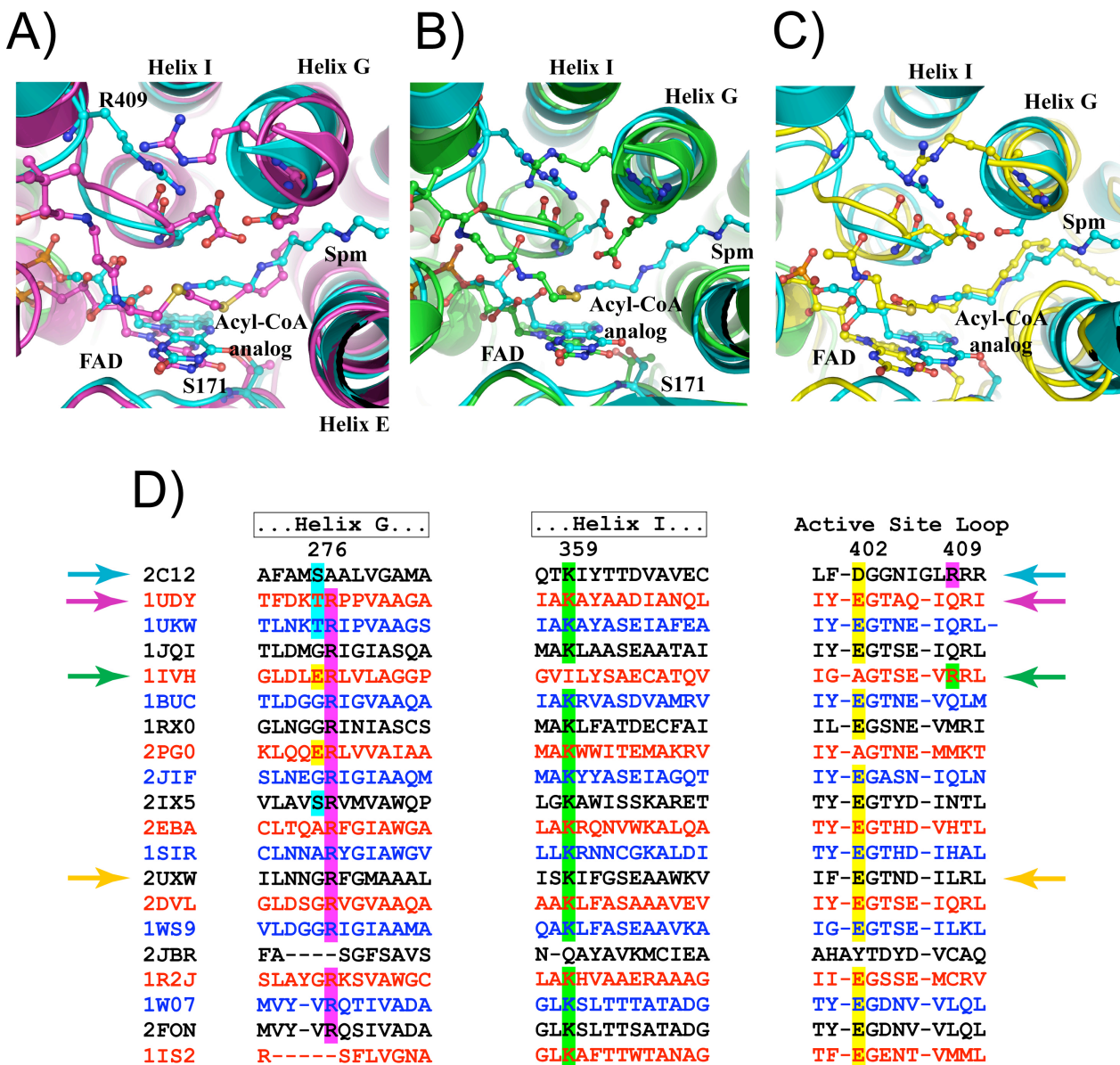


Fig. S2: Overlay of NAO and selected homologs. **A)** NAO (cyan, PDB code 2s12) superimposed with MCAD (magenta, PDB code 1udy); **B)** NAO superimposed with isovaleryl-CoA dehydrogenase (green, PDB code 1ivh); **C)** NAO superimposed with human very long chain Acyl-CoA dehydrogenase (yellow, PDB code 2uxw). Shaded boxes correspond to residues in NAO that occupy the equivalent 3-dimensional space as Ser276 (cyan), Arg409 (magenta), Lys359 (green) and the active site base Asp402 (yellow). **D)** The secondary structure alignment (from the SSM web-server) for 20 homologs in the active site region of NAO illustrated in parts A-C. The numbering scheme corresponds to that of NAO (2C12). The full PDB titles are given below.

2C12:A Crystal Structure of Nitroalkane Oxidase in Complex with Spermine, A Competitive Inhibitor
 1UDY:A Medium-Chain Acyl-CoA Dehydrogenase with 3-Thiooctanoyl-CoA
 1UKW:A Crystal structure of medium-chain acyl-CoA dehydrogenase from *Thermus thermophilus* HB8
 1JQI:A Crystal Structure of Rat Short Chain Acyl-CoA Dehydrogenase Complexed with Acetoacetyl-CoA
 1IVH:A Structure of Human Isovaleryl-CoA Dehydrogenase: Structural Basis for Substrate Specificity
 1BUC:A Three-Dimensional Structure of Butyryl-CoA Dehydrogenase from *Megasphaera elsdenii*
 1RX0:A Crystal structure of isobutyryl-CoA dehydrogenase complexed with substrate/ligand
 2PG0:A Crystal structure of acyl-CoA dehydrogenase from *Geobacillus kaustophilus*
 2JIF:A Structure Of Human Short-Branched Chain Acyl-CoA Dehydrogenase (ACADSB)
 2IX5:A Short Chain Specific Acyl-CoA Oxidase from *Arabidopsis thaliana*, Acx4 in Complex with Acetoacetyl-CoA
 2EBA:A Crystal structure of the putative glutaryl-CoA dehydrogenase from *Thermus thermophilus*
 1SIR:A The Crystal Structure and Mechanism of Human Glutaryl-CoA Dehydrogenase
 2UXW:A Crystal Structure of Human Very Long Chain Acyl-CoA Dehydrogenase (ACADVL)
 2DVL:A Crystal structure of project TT0160 from *Thermus thermophilus* HB8
 1WS9:A Crystal structure of project ID TT0172 from *Thermus thermophilus* HB8
 2JBR:A Monooxygenase Component of *p*-Hydroxyphenylacetate Hydroxylase from *Acinetobacter baumannii*
 1R2J:A Fkbl for Biosynthesis of Methoxymalonyl Extender Unit of Fk520 Polyketide Immunosuppressant
 1W07:A *Arabidopsis thaliana* Acyl-Coa Oxidase 1
 2FON:A X-ray crystal structure of LeACX1, an acyl-CoA oxidase from *Lycopersicon esculentum* (tomato)
 1IS2:A Crystal Structure of Peroxisomal Acyl-CoA Oxidase-II from Rat Liver