

Supporting Information

Structural and functional insights into aldosterone synthase interaction with its redox partner protein adrenodoxin Simone Brixius-Anderko¹ and Emily E. Scott^{1,2,#}

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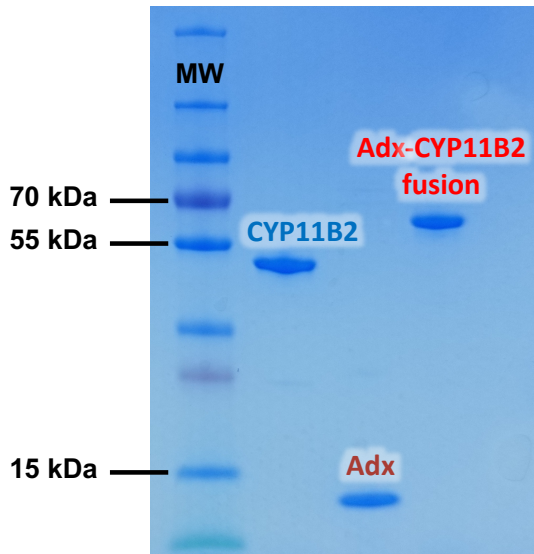


Figure S1: Protein purity by SDS-PAGE of purified proteins (CYP11B2, adrenodoxin, and adrenodoxin-CYP11B2 fusion protein) and molecular weight marker (left lane).

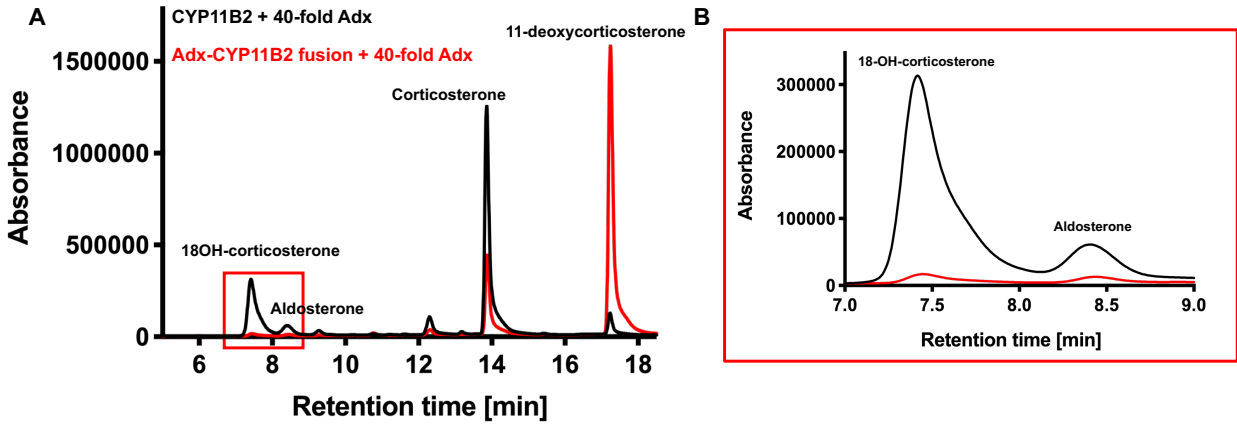


Figure S2: CYP11B2 catalysis. HPLC chromatogram of CYP11B2 (black line) and the adrenodoxin-CYP11B2 fusion protein (red line) conversion of 11-deoxycorticosterone to corticosterone, 18OH-corticosterone, and aldosterone (**A**) with focus on 18OH-corticosterone and aldosterone production (**B**).

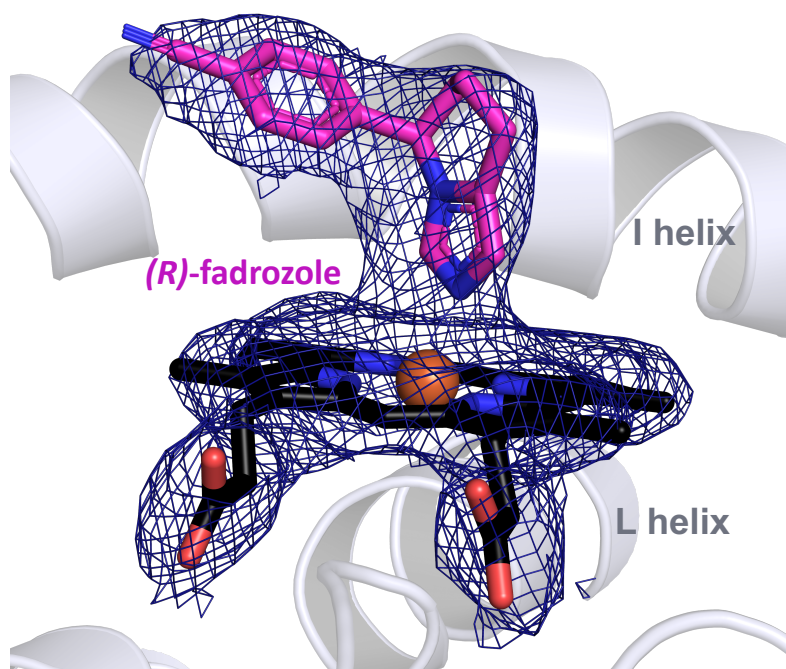


Figure S3: Detail of CYP11B2/(*R*)-fadrozole active site. The dark blue mesh shows electron density (simulated annealing/composite omit map) for the ligand (*R*)-fadrozole (magenta) and the heme prosthetic group in the CYP11B2 active site.

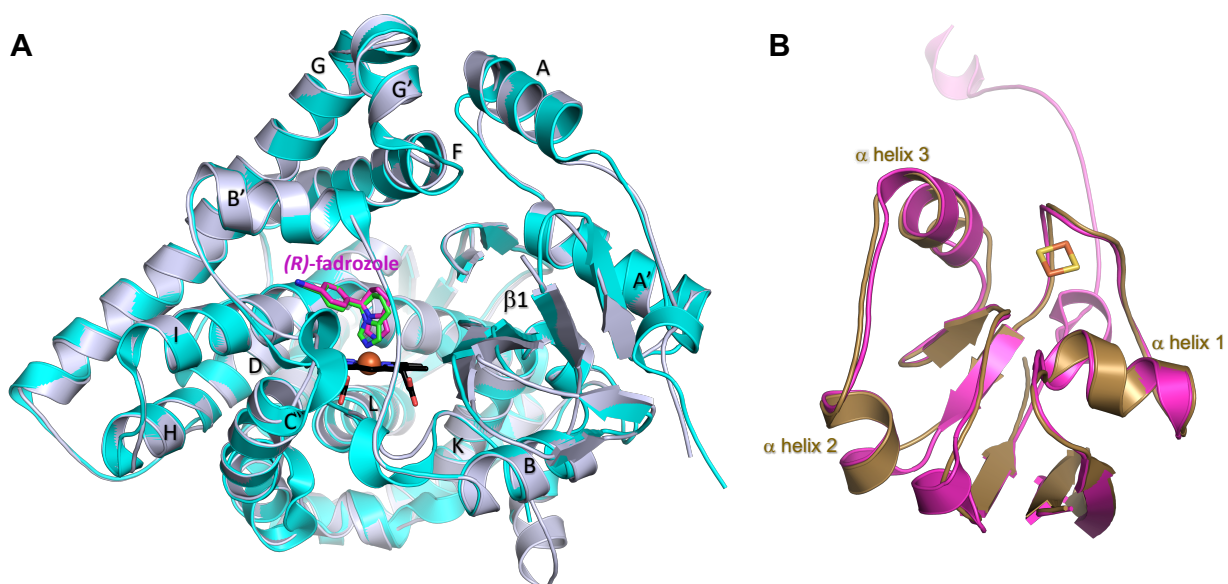


Figure S4: Comparisons of fused and isolated proteins reveal few structural changes. Comparison of CYP11B2 fused to adrenodoxin (light blue with *(R)*-fadrozole in magenta) with the isolated CYP11B2 enzyme (PDB 4FDH, cyan with *(R)*-fadrozole in green) yields a C α RMSD of 0.38 Å (A). Comparison of adrenodoxin fused to CYP11B2 (brown) with unfused adrenodoxin (PDB 3P1M, magenta) yields a C α RMSD of 0.53 Å (B).