

Supplementary Information for “Structural and spectroscopic characterization of a product Schiff-base intermediate in the reaction of the quinoprotein glycine oxidase, GoxA”

Running Title: CTQ-product Schiff-base

Dante Avalos^{1†}, Sinan Sabuncu^{2†}, Kyle J. Mamounis³, Victor L. Davidson³, Pierre Moënne-Loccoz² and Erik T. Yukl^{1}*

¹Department of Chemistry and Biochemistry, New Mexico State University, Las Cruces, NM 88003.

²Department of Biochemistry and Molecular Biology, School of Medicine, Oregon Health and Science University, Portland, OR 97239

³Burnett School of Biomedical Sciences, College of Medicine, University of Central Florida, Orlando, FL 32827

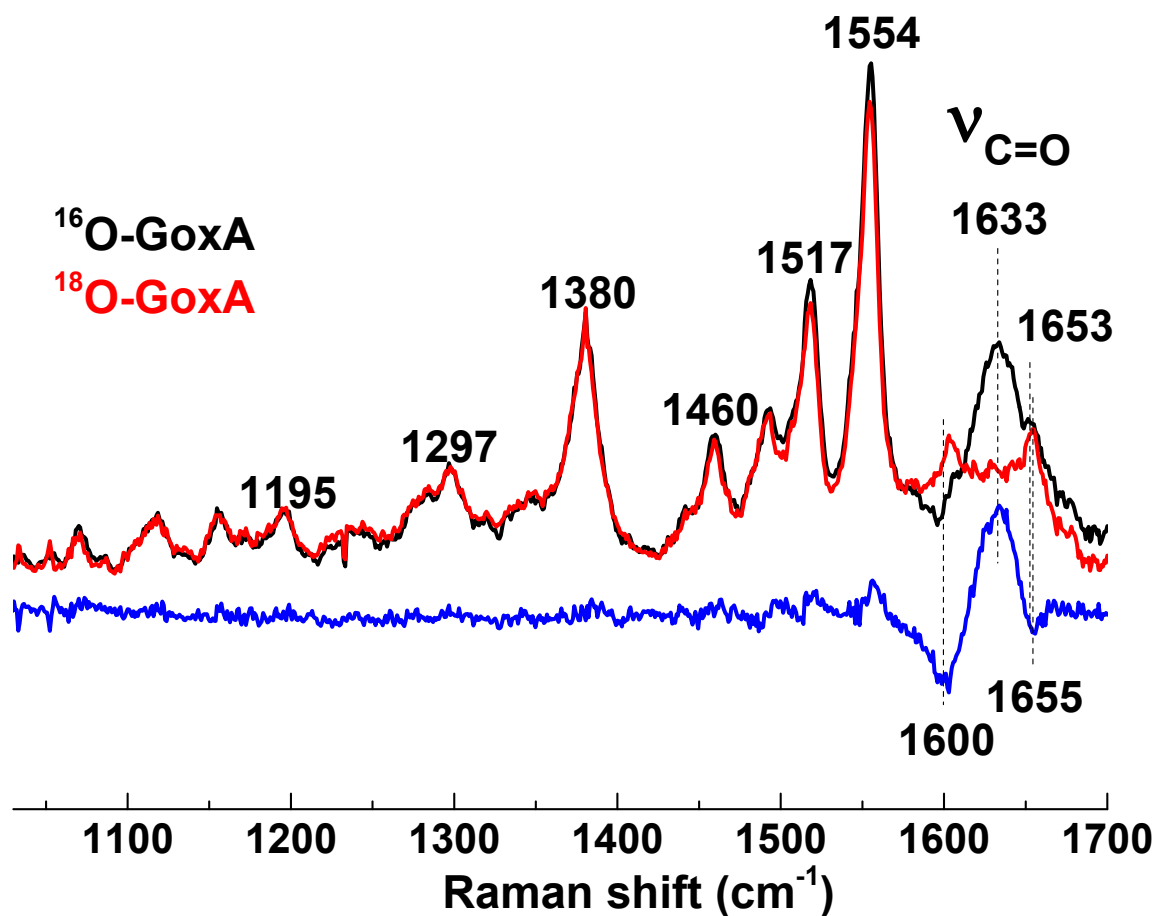


Figure S1. RR spectra of redox cycled PIgOx A obtained with 407 nm excitation at room temperature; the final protein concentration was $\sim 500 \mu\text{M}$ in unlabeled (black) or ^{18}O -water (red) after multiple turnover cycles with 5 mM Gly in 50 mM KPi pH 7.5 under a constant O_2 -saturated headspace.

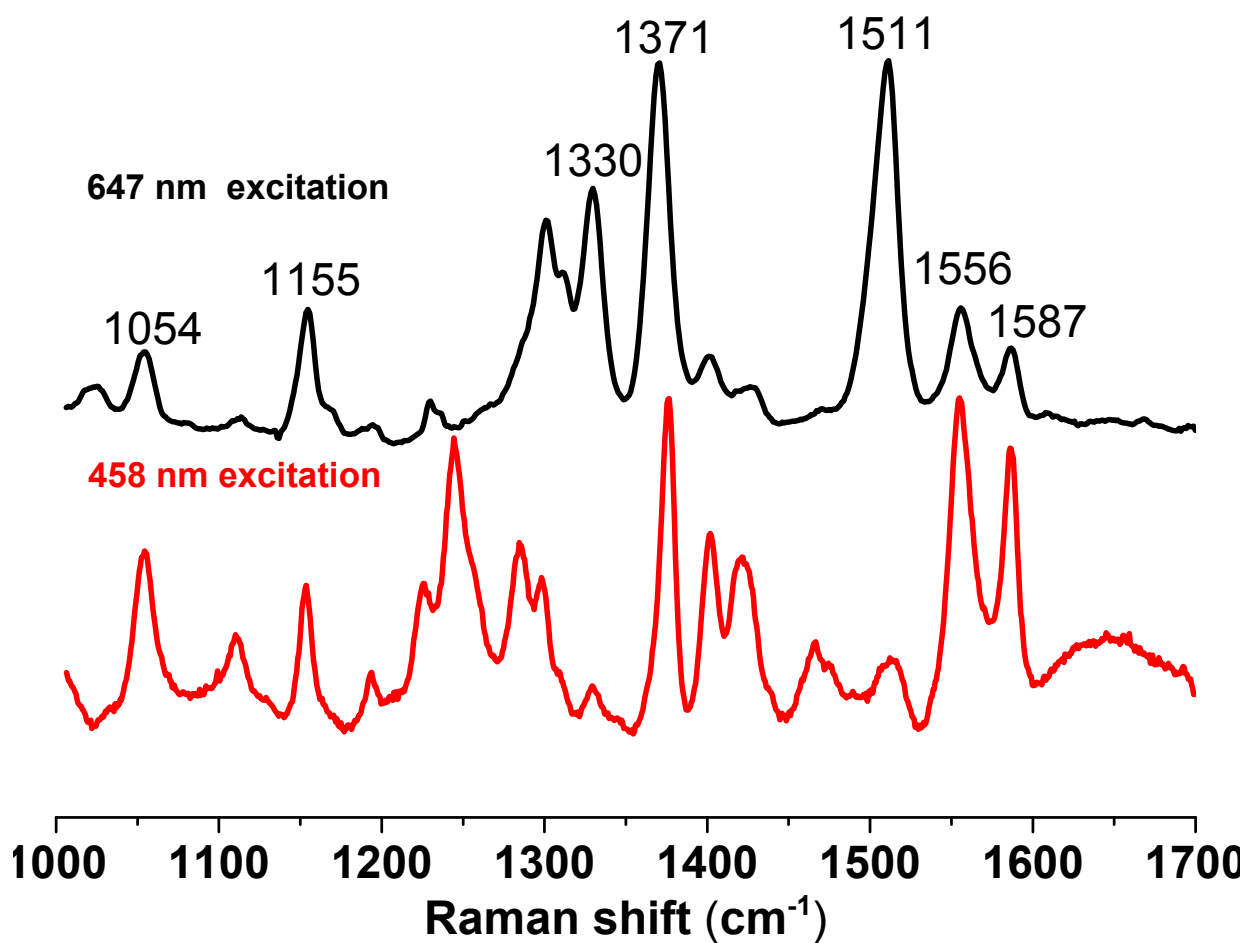


Figure S2. RR spectra of Gly-GoxA with 647nm excitation (black) and with 458nm excitation (red) at room temperature. The final protein concentration was $\sim 550 \mu\text{M}$ in 50 mM KPi pH 7.5. The spectra are normalized with respect to the 1371-cm⁻¹ band.

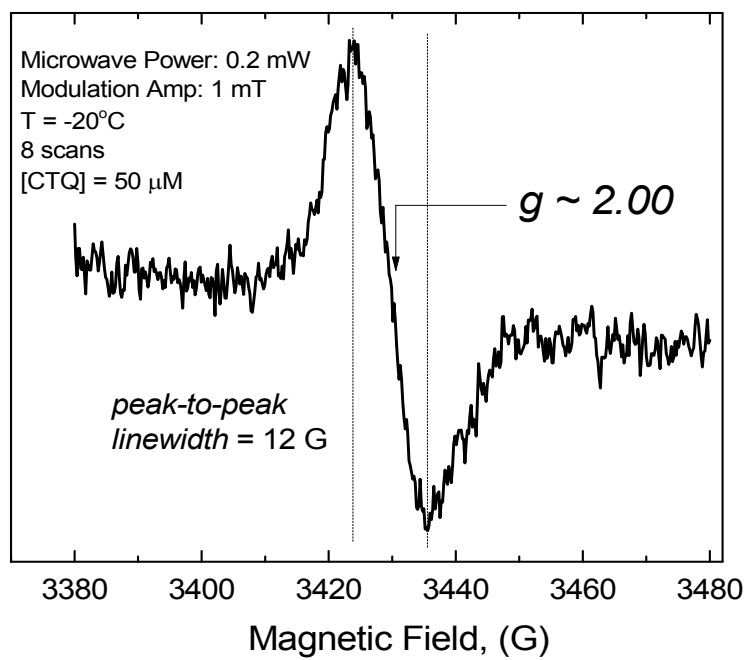


Figure S3. Residual organic radical signal observed in the EPR spectra of Gly-GoxA at $-20\text{ }^{\circ}\text{C}$.