

**Resonance Raman Characterization of the Peroxo and Hydroperoxo
Intermediates in Cytochrome P450**

Supporting Information

Ilia G. Denisov¹, Piotr J. Mak², Thomas M. Makris¹, Stephen G. Sligar^{1,3,4}, James R. Kincaid²

Department of Biochemistry¹, Chemistry³, and College of Medicine⁴, University of Illinois,
Urbana, IL 61801, and Department of Chemistry², Marquette University, Milwaukee, WI 53233

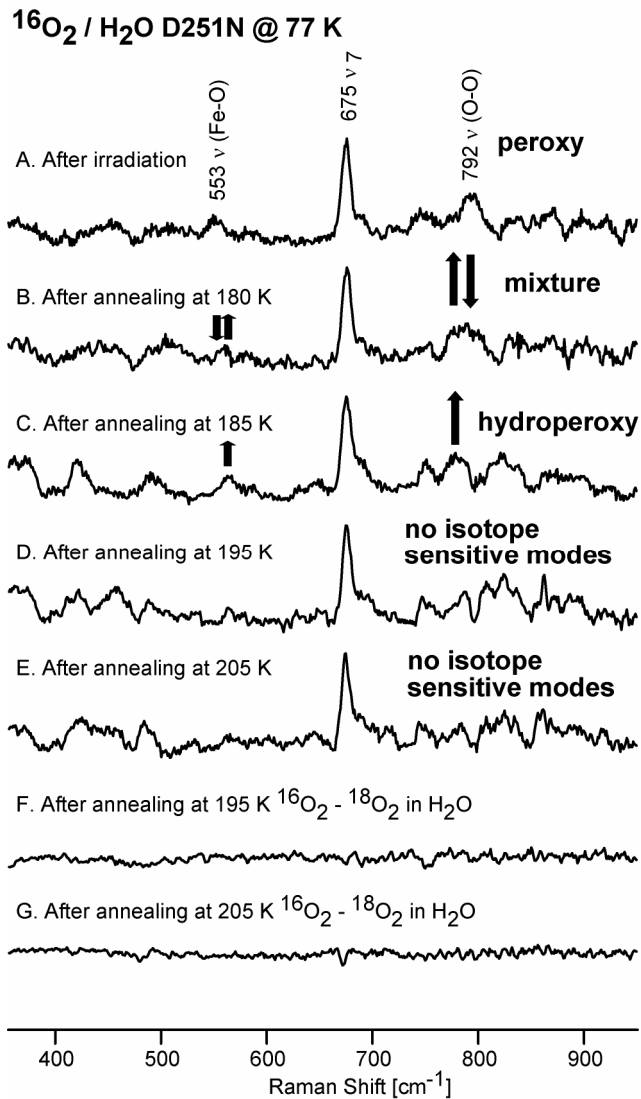


Figure S1. The resonance Raman spectra of irradiated and annealed at different temperature samples of D251N CYP101 in H_2O buffer: immediately after irradiation (A); after annealing at 180 K (B); after annealing at 185 K (C); after annealing at 195 K (D), and after annealing at 205 K (E). Two bottom traces shows difference spectra between $^{16}\text{O}_2 - ^{18}\text{O}_2$ in H_2O of the samples annealed at 195 K (F) and at 205 K (G) (excitation at 442, temperature 77 K).

Table S1. Calculated parameters of Fe-O-O in [4], [5a], and [5b]

| System | Fe-O, Å | O-O, Å | Fe-O-O, deg | Ref |
|--------|-----------------|------------|-------------|--------------------|
| [4] | 1.82-2.0 | 1.31-1.37 | | ¹ |
| [5a] | 1.99 | 1.41 | | “ |
| [5b] | 1.86-1.87(1.82) | 1.52(1.45) | | “ (²) |
| [4] | 1.94 | 1.32 | | ³ |
| [5b] | 1.80 | 1.44 | | |
| [4] | 1.95 | 1.31 | 119 | ⁴ |
| [5a] | 1.99 | 1.33 | 121 | |
| [5b] | 1.88 | 1.46 | 117 | |
| [4] | 1.81 | 1.29 | | ⁵ |
| [5a] | 1.92 | 1.31 | | |
| [5b] | 1.85 | 1.45 | | |
| [4] | 1.82 | 1.31 | | ⁶ |
| [5a] | 1.95 | 1.33 | | |
| [5b] | 1.89 | 1.46 | | |

References

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