Supplementary material for

NADH reduction of nitroaromatics as a probe for residual high-spin ferric form in a cytochrome P450

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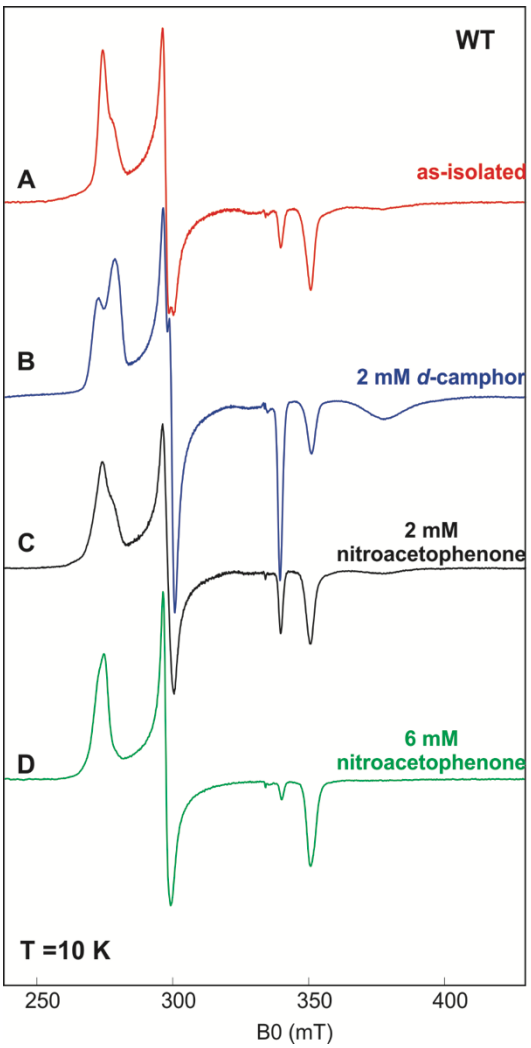

Figure S1. CW EPR spectra of WT CYP101A1 under different conditions. (A) 337 μM substrate free WT CYP101A1 (red trace "as isolated"), (B) 327 μM of WT CYP101A1 with 2 mM *d*-camphor **1** (blue trace), bottom, (C) 331 μM of WT CYP101A1 with 2 mM nitroacetophenone **6** (black trace), (D) 320 μM of WT CYP101A1 with 6 mM nitroacetophenone **6** (green trace). Experimental conditions: temperature 10 K, microwave power = 2 mW, microwave frequency = 9.384 GHz, modulation amplitude = 1 mT.

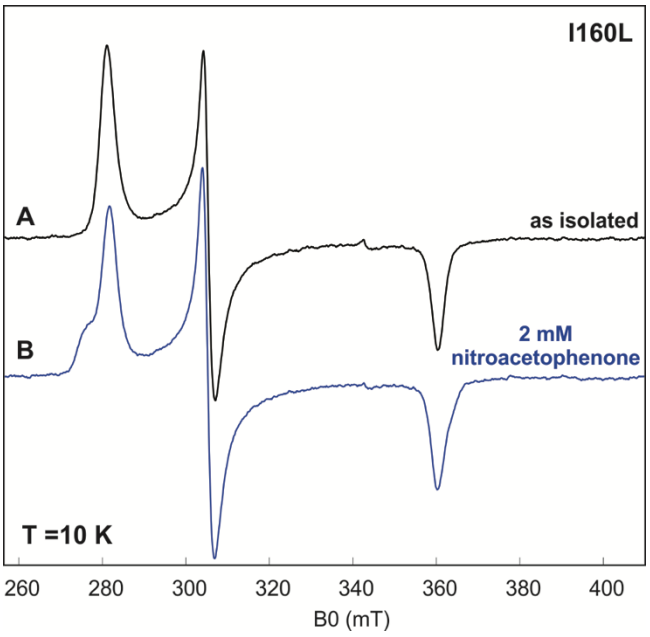

Figure S2. CW EPR spectra of I160L CYP101A1 under different conditions. (A) 300 μM of substrate-free I160L CYP101A1 (B) 300 μM uM of I160L CYP101A1 with 2 mM *m*-nitroacetophenone **6**. Experimental conditions: temperature 10 K, microwave power = 2 mW, microwave frequency = 9.625 GHz, modulation amplitude = 1 mT.

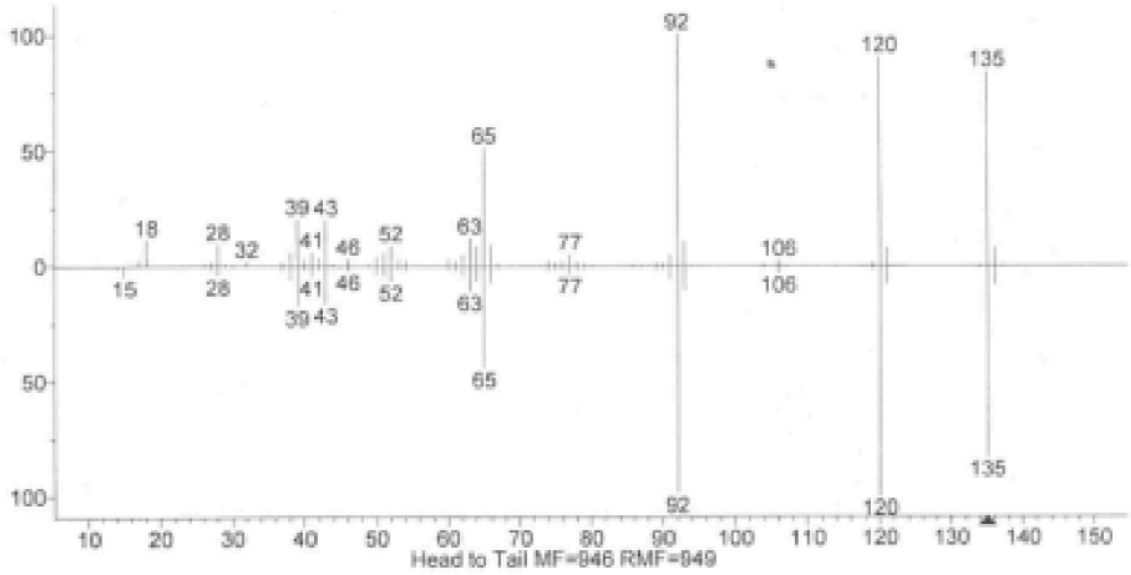

Figure S3. Comparison of mass spectrum of Nrase product **7a** (top) with that of genuine *m*-aminoacetophenone (bottom).

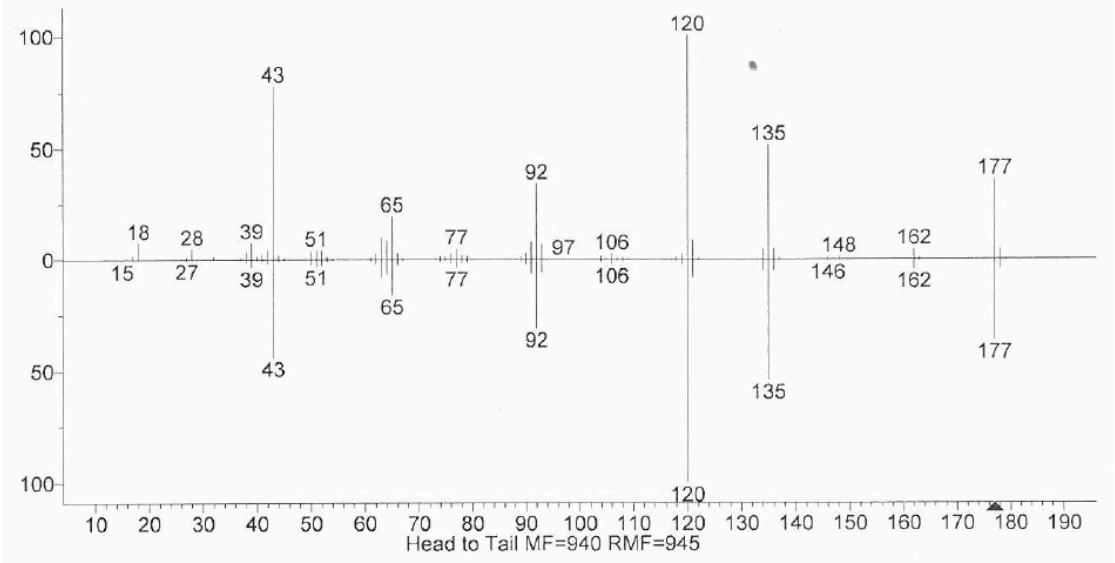

Figure S4. Comparison of mass spectrum of post-column product **7b** (top) with that of genuine *m*-(N-acetyl)-aminoacetophenone (bottom)