Electronic Supplementary Information

Hydroxyl radical generation *via* photoreduction of a simple pyridine *N*-oxide by an NADH analogue

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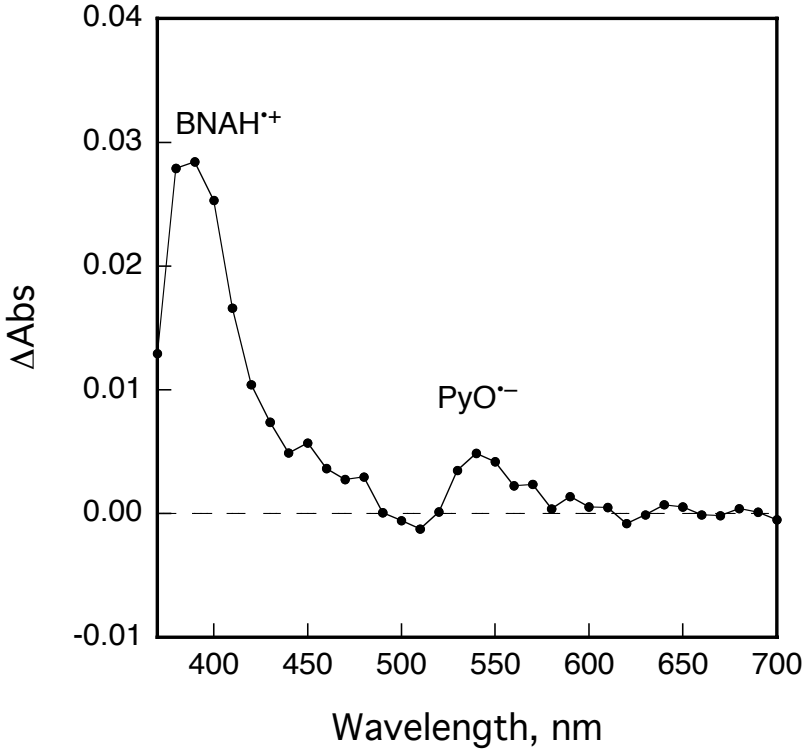

Fig. S1 Transient absorption spectra observed by photoexcitation of a deaerated MeCN solution of BNAH (3.5×10^{-5} mol dm^{-3}) and PyO (1.0×10^{-1} mol dm^{-3}) at 4 μs after laser excitation (λ_{ex} = 355 nm) at 298 K.

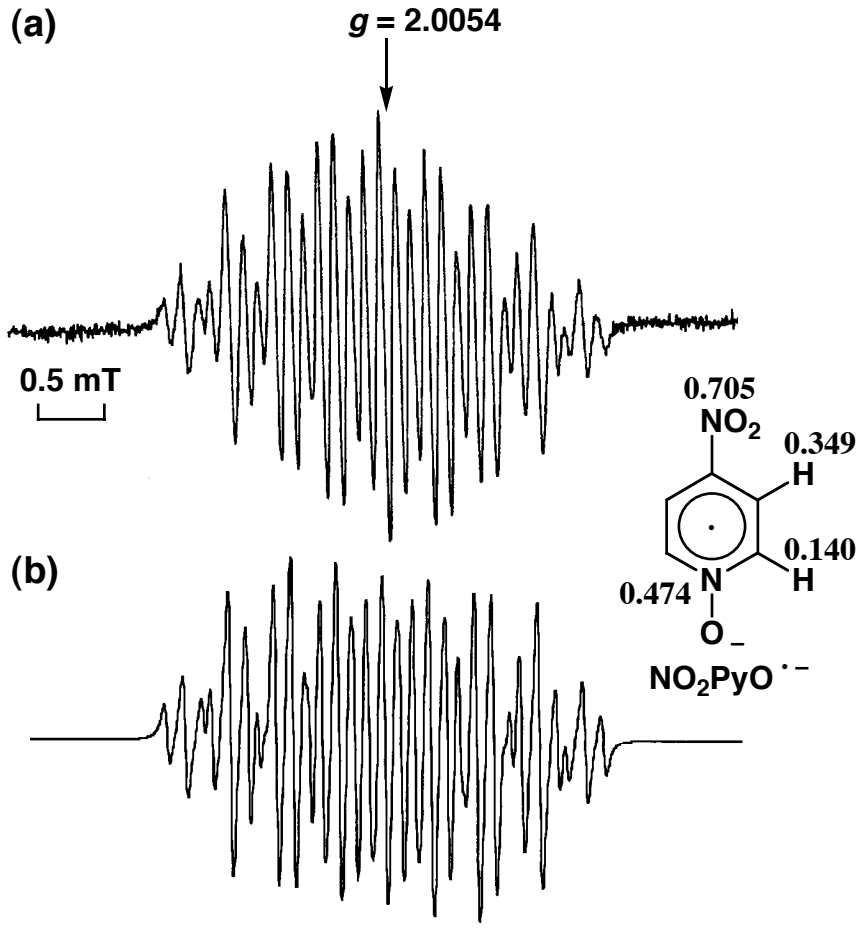

Fig. S2. (a) EPR spectrum of $NO_2PyO^{\bullet-}$ generated by irradiation of a deaerated MeCN solution of NO_2PyO (1.0×10^{-3} mol dm^{-3}) and BNAH (1.0×10^{-3} mol dm^{-3}) at 298 K. (b) The computer simulation spectrum with the hfc values (in mT).

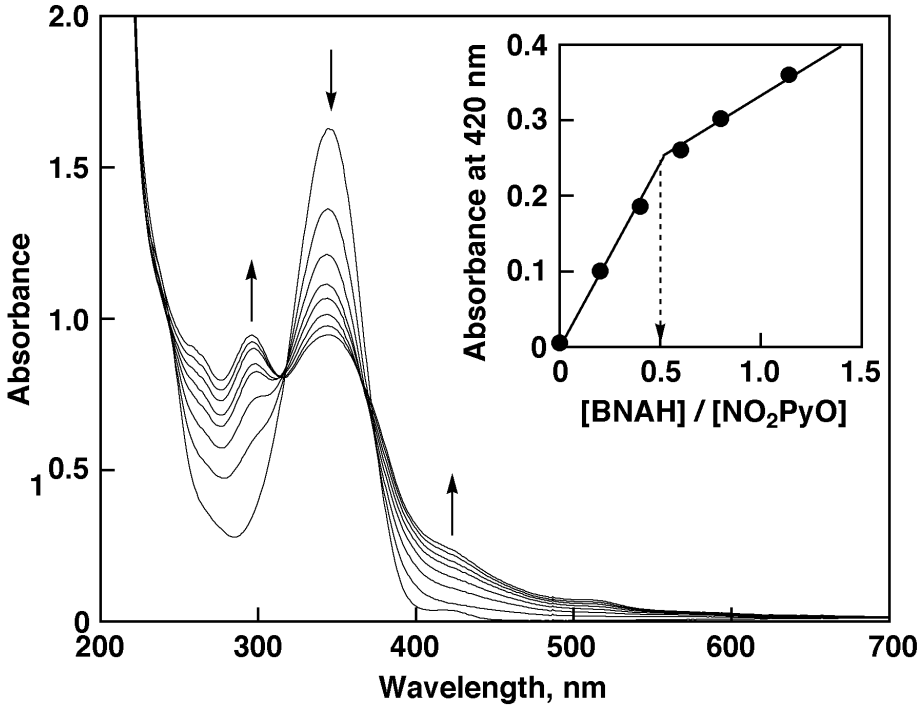

Fig. S3. Spectral change observed in the reaction of NO_2PyO (5.0×10^{-5} mol dm^{-3}) with BNAH (5.0×10^{-4} mol dm^{-3}) in deaerated MeCN under irradiation at $\lambda = 340$ nm at 298 K.

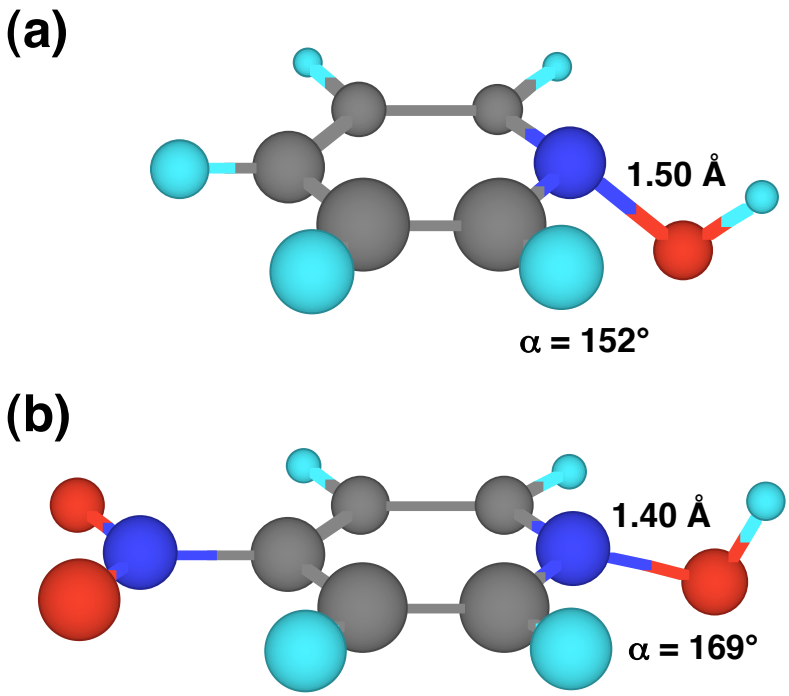

Fig. S4. B3LYP/6-31G* minimized structures of (a) PyOH$^{\bullet}$ and (b) NO_2PyOH$^{\bullet}$ with the calculated nitrogen–oxygen bond distances and the out-of-plane bending angles, α.