Interplay of nucleophilic catalysis with proton transfer in the nitrile reductase QueF from *Escherichia coli*

Jihye Jung^{a,b}, Jan Braun^a, Tibor Czabany^{a,b} and Bernd Nidetzky^{*a,b}

^a Institute of Biotechnology and Biochemical Engineering, Graz University of Technology, NAWI Graz, Petersgasse 12/1, A-8010 Graz, Austria

E-mail: bernd.nidetzky@tugraz.at; Fax: +43 316 8738434; Tel.: + 43 316 8738400

^b Austrian Centre of Industrial Biotechnology, Petersgasse 14, A-8010 Graz, Austria



Fig. S1 Protein mass spectrum of ecQueF D197H variant after incubation with $preQ_0$. An asterisk on peaks indicates the $preQ_0$ -bound enzyme complex. The enzyme solution with $preQ_0$ was prepared and analyzed as described in the section "Experimental" of the main text. Procedures from our earlier study of wildtype ecQueF were used.¹ The deconvoluted data is shown in Fig. 2 of the main text.

References

1 J. Jung, T. Czabany, B. Wilding, N. Klempier and B. Nidetzky, *J. Biol. Chem.*, 2016, **291**, 25411–25426.