SUPPORTING MATERIAL 1/22/12

Role of Coupled-Dynamics in the Catalytic Activity of Prokaryotic-like Prolyl-tRNA Synthetases

Brianne Sanford[†$], Bach Cao[†], James M. Johnson[†], Kurt Zimmerman[†], Alexander M. Strom[†], Robyn M. Mueller[†], Sudeep Bhattacharyya[†*], Karin Musier-Forsyth[$*], and Sanchita Hati[†*]

[†]Department of Chemistry, University of Wisconsin –Eau Claire, WI, 54702

[$]Department of Chemistry and Biochemistry, Center for RNA Biology, The Ohio State University, Columbus, OH, 43210

[*]To whom correspondence should be addressed: S.B.: phone: 715-836-2278; fax: 715-836-4979; email: bhattas@uwec.edu; K.M.F.: phone: 614-292-2021; fax: 614-688-5402; email: musier@chemistry.ohio-state.edu ; S.H.: phone: 715-836-3850; fax: 715-836-4979; email: hatis@uwec.edu.

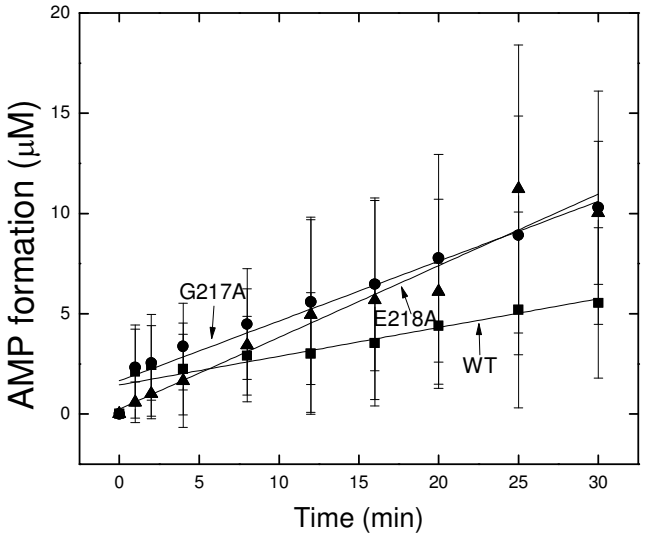
SUPPLEMENTAL FIGURE LEGENDS

Figure S1. a) Pre-transfer editing reaction in the presence of cognate proline by WT, G217A, and E218A Ec ProRS. The editing activity was monitored by quantifying the amount of AMP formed at 37 °C using 0.5 μM enzyme and 30 mM proline. b) Deacylation of Ala-tRNA^{Pro} by WT, G217A, and E218A Ec ProRS. Reactions were initiated by the addition of enzyme to a final concentration of 5 μM (based on active site titration). Deacylation in the presence of buffer is also shown.

Figure S2. Computed RMSPs (see eq. 5 of main text) for the eigenvectors 1-10 using 5-ns simulation data. RMSPs of the PBL were obtained using the modeled structure of Ec ProRS as described in the main text; WT (black, solid line), G217A (gray, solid line) and E218A (black, broken line) Ec ProRS.

Fig. S1.

a)


AMP formation (μM)
Time (min)
G217A
E218A
WT

b)

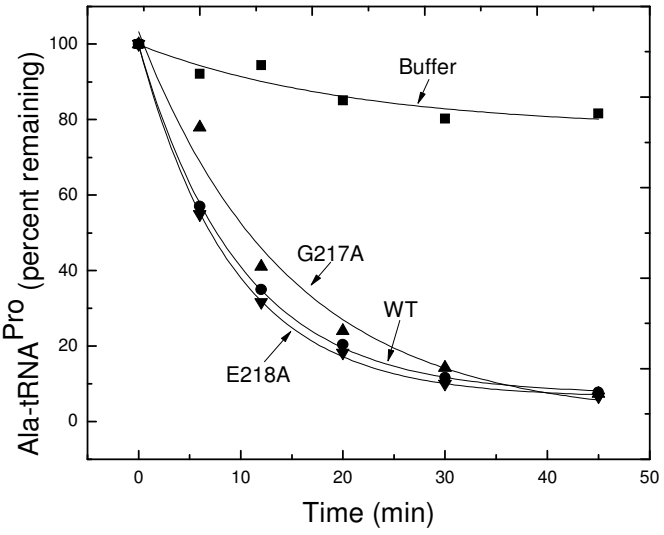

Ala-tRNA^{Pro} (percent remaining)
Time (min)
Buffer
G217A
WT
E218A

Fig. S2.