

Multiple Pathways Promote Dynamical Coupling between Catalytic Domains in *Escherichia coli* Prolyl-tRNA Synthetase

James M. Johnson[†], Brianne L. Sanford[§], Alexander M. Strom[†], Stephanie N. Tadayon[†], Brent P. Lehman[†], Arrianna M. Zirbes[†], 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. Dynamic cross-correlations between the C_{α} atoms of Ec ProRS obtained from the cluster analysis and PCA. A value of +1.0 was set for strongly correlated motion and is colored red, whereas -1.0 was used for strongly anti-correlated motions and is colored blue. The abbreviations used are: CD, catalytic (aminoacylation) domain; INS, insertion domain; and ACB, anticodon binding domain.

Figure S2. Conserved residues from SCA. A normalized plot of ΔG_i^{stat} vs. position (residue number). A value of 1 indicates 100% conservation over the 452 sequences examined.

Table S1. List of primers used in this study, bold letters represent the sites of mutation.

1.	ProRS_D198At: 5'-GCGCCGTACAAGCC GCC ACCGGTTCTATCGGCGG-3'
	ProRS_D198Ab: 5'-CCGCCGATAGAACCGGT GGCGG CTTGTACGGCGC-3'
2.	ProRS_E234At: 5'-GCAGCGAACATT GCA CTGGCAGAAGC-3'
	ProRS_E234Ab: 5'-GCTTCTGCCAGT GCA ATGTTCTGCTGC-3'
3.	ProRS_H302At: 5'-GCGCGGTGAT GCC GAGCTGAACG-3'
	ProRS_H302Ab: 5'-CGTTCAGCTC GGC ATCACCGCGC-3'
4.	ProRS_N305At: 5'-CGAGCT GGCC GAAGTTAAAGC -3'
	ProRS_N305Ab: 5'-GCTTTAACTTC GGCC AGCTCG- 3'
5.	ProRS_G412At: 5'-CGTGGTATCGAAGTT GCT CACATCTTCCAGCTGGG-3'
	ProRS_G412Ab: 5'- CCCAGCTGGAAGATGT GAGCA ACTTCGATACCACG-3'
6.	ProRS_F415At: 5'-GGTCACATC GCCC AGCTGGG-3'
	ProRS_F415Ab: 5'-CCCAGCT GGGC GATGTGACC-3'

Fig. S1

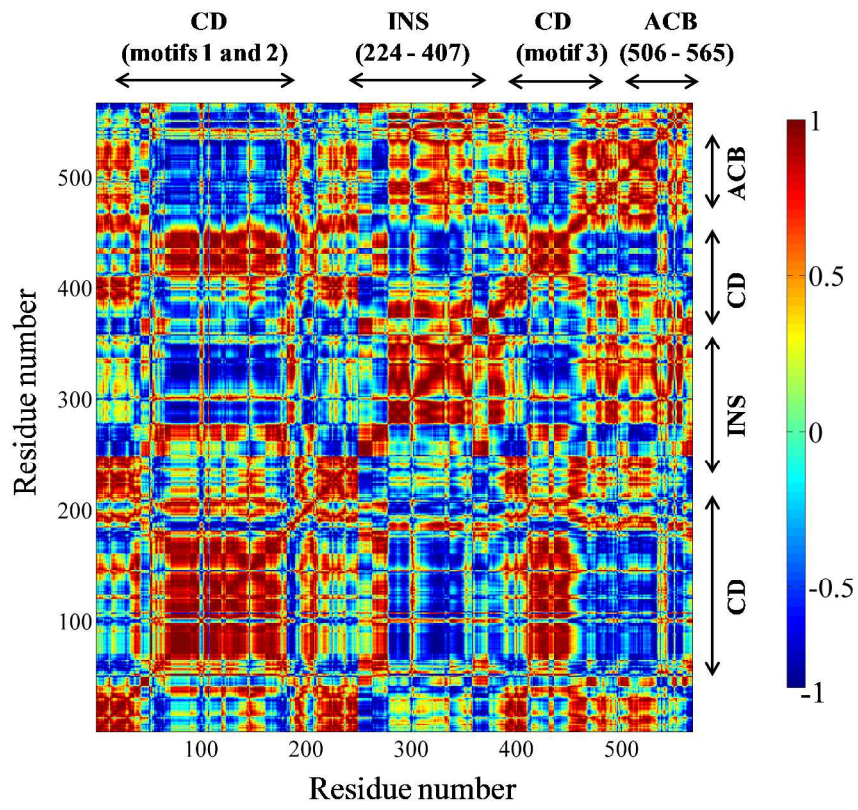


Fig. S2

