

## Role of Coupled-Dynamics in the Function of Prokaryotic-like Prolyl-tRNA Synthetases

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Prolyl-tRNA synthetases (ProRSs) are class II synthetases that catalyze covalent attachment of proline (Pro) to the 3'-end of tRNA<sup>Pro</sup> as a part of polypeptide building, during translation. Previous experimental studies have shown that the existence of the editing domain is important for the cognate amino acid activation by *E. coli* ProRS. In the absence of the editing domain, the overall activation efficiency is decreased by ~ 1,200-fold (1). It is still unclear how the editing domain influences the catalytic activity. To better understand the role of the editing domain in amino acid activation, the prokaryotic-like *Enterococcus faecium* ProRS was studied through molecular dynamics (MD) simulations. The two systems: the full-length enzyme and the editing domain deletion mutant were used for this study. In particular, targeted Molecular Dynamics (tMD) was used to observe the transition of the proline-binding loop from the open conformation to the closed (substrate-bound) conformation. Herein, we will report the influence of neighboring structural elements on the dynamics of the proline-binding loop and evaluate the importance of the editing domain on catalytic process.

### Reference:

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