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Role of microsecond structural dynamics of a small RNA ($preQ_1$ riboswitch) in bacterial gene expression

DNA, RNA, and proteins are dynamic macromolecules that perform various cellular functions, such as gene expression, enzymatic reaction, catalysis, etc. which are essential for the existence of 'life'. Among these, gene expression (i.e., synthesis of nascent DNA, RNA, and proteins) is generally regulated by proteins and only sometimes by RNA. Riboswitches are small RNA elements that regulate gene expression in lower organisms, such as bacteria. This regulation process is primarily driven by the structural change of the riboswitch upon binding of specific cellular metabolites. The prequeuosine ($preQ_1$) riboswitch from *Bacillus subtilis* regulates gene expression at the transcription (i.e., DNA to mRNA synthesis) stage. In this presentation, I will discuss our recent results of the state-of-the-art single-molecule fluorescence spectroscopy, namely, two-dimensional fluorescence lifetime correlation spectroscopy (2D FLCS),[1] measurements on the ligand-binding 'aptamer domain' of $preQ_1$ riboswitch which revealed its folding-unfolding energy landscape and provided a molecular picture of the bacterial transcription regulation process.[2] 2D FLCS distinguishes the conformers of a biopolymer using their fluorescence lifetimes and provides their interconversion dynamics with a microsecond time resolution. Our results suggest that the aptamer domain undergoes folding-unfolding dynamics involving three states in a wide time range from a microsecond to >10 milliseconds. It is also observed that the aptamer domain binds to the ligand ($preQ_1$) and co-factor (Mg^{2+}, which helps in RNA folding) with two distinct mechanisms, induced-fit and conformational selection, respectively. The molecular picture obtained from the observed results indicate that the microsecond folding-unfolding dynamics of the aptamer domain and the ligand binding through induced-fit mechanism are crucial for $preQ_1$ riboswitch to regulate bacterial transcription kinetically.

References

（1） K. Ishii, and T. Tahara, *J. Phys. Chem. B* **117**, 11414-11422 & 11423-11432 (2013).

（2） B. Sarkar, K. Ishii, and T. Tahara, *J. Am. Chem. Soc.* **143**, 7968-7978 (2021).