Conformational Changes in the Bacterial Translocase Subunit SecA

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P–A3–01

MOLECULAR DYNAMICAL THEORY FOR SPONTANEOUS EMISSION OF BIO – PHOTONS IN THE LIVING SYSTEMS

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Purpose: Many experiments show that the bio – photon emission including thermal radiation and γ – photons of the Living systems is a general and important biological phenomenon. We propose here a theory of moleculur biology for the emission of bio – photons .

Methods: We think that the bio – photon emission come from the transition of bonding electrons and displacement of active nuclei and non – linear vibration of molecular chains resulting from the solitons excited by the intramolecular localized fluctuation and the deformation of structure and conformation of molecular chains caused by the energy released in ATP hydrolysis in biomacromolecules with biological temperature. The Hamiltonian and Wave function in our theory are

$$H=\sum_i\left[\frac{1}{2m}p_i^2+\frac{m}{2}\omega_0^2r_i^2-\frac{m\omega_1^2}{2}r_ir_{i+1}\right]+\sum_i\left[\frac{M}{2}\dot{R}_i^2+\frac{1}{2}\lambda(R_i-R_{i-1})^2\right.$$

$$\left.-\frac{\lambda_1}{3}(R_i-R_{i-1})^3\right]+\sum_i\left[\frac{m\chi_1}{2}(R_{i+1}-R_{i-1})r_i^2+m\chi_2(R_{i+1}-R_i)r_ir_{i+1}\right],$$

$$|\Phi>=\frac{1}{\lambda}\sum_i(1+\varphi_i(t)b_i^+)\exp\left[\sum_q(\alpha_{q_i}(t)a_q^+-\alpha_q^*(t)a_q)\right]\pi_q\frac{(a_q^+)^{n_q}}{\sqrt{n_q!}}|0>$$

Results: applying non – linear quantum theory we find out the Intensity of bio – photon emission to be

$$W=\frac{256\lambda_1^2z_0^4g\hbar^2\bar{A}\omega'\beta'N'\omega^3}{9M^2V_0^4v^2(\vec{P}\cdot\vec{e}_q)^2g_mC^3\bar{G}(\omega)}\left[-\vec{M}(\vec{x})J_1(\vec{x})-(\vec{x}\cdot\vec{M}(\vec{x})\right.$$

$$\left.-\vec{M}(\vec{x}))J_2(\vec{x})\right]\mathrm{Sin}^2((\tilde{\omega}_0-\omega)t/2)/(\tilde{\omega}_0-\omega)^2\{[[A^2(T)\mathrm{Cos}^2(\tilde{E}th$$

$$(v(vt-x_0)))]f_0(\tilde{E})+\frac{\tilde{E}^2ch^2\frac{1}{2}+1}{2v(\tilde{E}^2+1)}\Big]^2+A^4(T)f_0(\tilde{E})\mathrm{Sin}^2(\tilde{E}th(v$$

$$(vt-x_0)))\}\exp\left|-\sum_q\frac{(\vec{P}\cdot\vec{e}_q)^2}{2MN\hbar\omega_q}\mathrm{Cth}\left(\frac{\hbar V_0q}{2K_BT}\right)\right|$$

Condiusions: with the help of this result, we can explain all phonomena and properties of bio – photon emission obtained from experiments.

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CONFORMATIONAL CHANGES IN THE BACTERIAL *TRANSLOCASE* SUBUNIT SECA

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The homodimeric SecA protein is the peripheral subunit of the preprotein *translocase* in bacteria. It binds the preprotein and promotes its translocation across the bacterial cytoplasmic membrane by nucleotide modulated co-insertion and de-insertion into the membrane. SecA has a high affinity nucleotide binding site (NBS-I) in its amino terminal domain and a low affinity NBS (II) in its carboxy-terminal domain. The conformations of the nucleotide bound states of SecA were studied by site directed tryptophan fluorescence spectroscopy, tryptic digestion, differential scanning calorimetry and dynamic light scattering. SecA unfolds as a two domain protein. ADP binding to NBS-I increases the interaction between these domains, whereas the non-hydrolysable ATP analog AMP-PNP does not influence this interaction. ADP binding to both sites induces a more compact state, which is though to resemble the membrane de-inserted state of SecA. AMP-PNP induces a more extended conformation, which could resemble the membrane inserted state.

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PHOTOSENSING IN EUBACTERIA: *TRANS/CIS* ISOMERIZATION OF THE CHROMOPHORE OF PYP

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Purpose: Photoactive yellow protein (PYP) is a cytosolic eubacterial blue-light photosensor with a rhodopsin-like photocycle. The photochemical basis of the photocycle of PYP has been investigated to find a rationale for the high similarity of its photocycle to that of sensory rhodopsins, in spite of great structural differences.

Methods: The *p*-coumaric acid chromophore was extracted from the ground state of PYP (pG) as well as from the blue-shifted photocycle intermediate (pB). Extracts were analyzed by zone capillary electrophoresis and ^{1}H-NMR spectroscopy.

Results: Analysis of the chromophore extracts from pG and pB demonstrated that the chromophoric group of PYP isomerizes from *trans* to *cis p*-coumaric acid while progressing through the photocycle.

Conclusions: These results contribute to the understanding of the similarity in photocycle between PYP and sensory rhodopsins and show that also in Bacteria, so in all three domains of life, photosensing occurs by a common photochemical basis: isomerization of a chromophore double bond.

P–A3–04

CONFORMATIONS OF PROLINE DIPEPTIDE STUDIED BY AB INITIO METHOD

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Purpose: The low-energy conformations of trans- and cis-Ac-Pro-NHMe with down and up puckerings are studied in order to investigate the preference of the puckering of pyrrolidine ring for the preceding imide bond.

Methods: All ab initio calculations were carried out using the Gaussian 90 and 92 molecular orbital packages. Full geometry optimizations were performed at the direct HF/SCF level with the 6-31G** basis set. Single-point MP2 calculations were also performed on the optimized conformations with the same basis set.

Results: The intramolecularly hydrogen-bonded C7 conformer is found to be most preferred. The down puckering seems to be about 1.5 kcal/mol more stable than the up puckering at the HF/6-31G** and MP2/6-31G** levels. The optimized structural parameters are in general consistent with X-ray structures of peptides.

Conclusions: The preference and population for down and up puckered structures with the trans and cis imide bonds calculated here agree reasonably with the results obtained from the analysis of X-ray structures of proteins. The degree of puckering for each conformer is well described by puckering amplitudes.