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（For JSPS Fellow）

Form B-5

Date（日付）15.06.2014（Date/Month/Year：日/月/年）

Activity Report -Science Dialogue Program-

（サイエンス・ダイアログ事業　実施報告書）

- Fellow's name（講師氏名）: Krah, Alexander（ID No. P13705）

- Participating school（学校名）: Kyoto Prefectural Yamashito High School

- Date （実施日時）: 07.06.2014　　（Date/Month/Year:日/月/年）

- Lecture title（講演題目）: Mechanistic insights into the regulatory mechanism of the subunit from bacterial F-type ATP synthases

- Lecture summary（講演概要）: Please summary your lecture 200-500 words.

The talk contained three parts. In the first part I introduced Germany, summarizing the history and the nature. Additionally I gave impressions about the German culture and daily life in Germany, pointing out differences from the experience I had in Japan during my stay.

In the second part I gave a critical view on the decision why to become a scientist and compared this option with a career in industries (from a German perspective). I pointed out advantages and disadvantages for both choices and recommended neither choice. Students should make this decision by themselves depending on their own aptitudes.

In the last section I was talking about my current research. First I gave a brief introduction of the method I am using (Molecular Dynamics simulations) and how this method can give insights into biological questions. In the biological introduction I shortly explained why we need ATP (energy source) and how bacteria and mammals avoid the waste of ATP, concerning the hydrolysis mechanism in ATP synthases, after I explained how the molecular motor (ATP synthase) works. Due to a distinct inhibition mechanism, I explained why this research might be beneficial. In the result section, I showed how we can predict the ATP binding site of the ε subunit from thermophilic *Bacillus* PS3 (which is still under progress) based on the simulation of the biologically relevant monomer, while the crystal structure was obtained in a dimer, where the ATP molecule (monomer 1) is coordinated by two residues of monomer 2 (protein). Additionally, I showed that we could identify the Mg^{2+} binding site in the ε subunit from *Bacillus subtilis*, which has been shown to reduce ATP binding in the whole ATP synthase complex by ~500 fold. Using sequence alignment of the ε subunit from pathogenic bacteria, I proposed that in some ε subunits from pathogenic bacteria a Mg^{2+} binding site motif might be present, revealing a novel drug target. In addition I pointed out that site directed mutations (abolishing Mg^{2+} dependency) might enable structural characterization (crystallization) of Mg^{2+} dependent ε subunits from F-type ATP synthases.

- Language used（使用言語）: English

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- Lecture format（講演形式）:

◆Lecture time（講演時間）~60 min（分）, Q&A time（質疑応答時間） ~30 min（分）

◆Lecture style（ex.: used projector, conducted experiments）

（講演方法（例:プロジェクター使用による講演、実験・実習の有無など））

Power Point (use of projector)

◆Interpretation（ex.: assistance by accompanied person, provided Japanese explanation by yourself）（通訳（例:同行者によるサポート、講師本人による日本語説明））

No interpreter available

◆Name and title of accompanied person（同行者 職・氏名）

◆Other note worthy information（その他特筆すべき事項）:

- Impressions and opinions from accompanied person（同行者の方から、本事業に対する意見・感想等がありましたら、お願いいたします。）: