[Title of collaboration research]: NMR Study of Biomolecules

[The members of collaboration research]:

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[Reference home-page address]: http://www.jaist.ac.jp/nmcenter/labs/s-ohki-www/

[Other references]: (1) K.Murakami, F.Yumoto, S.Ohki, T.Yasunaga, M.Tanokura & T.Wakabayashi. (2005) "Structural Basis for Ca²⁺-regulated Muscle Relaxation at Interaction Sites of Troponin with Actin and Tropomiosin" *J. Mol. Biol.* **352**, 178-201. (2) H.Kurita, M.Nakatomi, H.Shimahara, M.Yazawa & S.Ohki. (2005) "Al³⁺ Binding Sites of Calmodulin and Its Effect on the Target Binding of Calmodulin" *Biochem. Biophys. Res. Commun.* **330**, 1060-1065. (3) S.Ohki, M.Eto, R.Takada, M.Shimizu, D.L. Brautigan & M.Kainosho (2003) "Distinctive Solution Conformation of Phosphatase Inhibitor CPI-17 Substituted with Aspartate at the Phosphorylation-site Threonine Residue" *J. Mol. Biol.* **326**, 1539-1547. (4) S.Ohki, M.Eto, E.Kariya, T.Hayano, Y.Hayashi, M.Yazawa, D.L. Brautigan & M.Kainosho. (2001) "Solution NMR Structure of the Myosin Phosphatase Inhibitor Protein CPI-17 Shows Phosphorylation-induced Conformational Changes Responsible for Activation" *J. Mol. Biol.* **314**, 834-849.

[Contents]

Biomolecules are well-organized nanomaterials. Their structures and dynamics are specialized for their functions and activities. Thus, study on structure-function relationship of biomolecules is essential to understand a wide variety of biological events. Furthermore, the knowledge obtained through the research works will give a clue to design new nanomaterials.

In our group, interest is focused on the proteins related to signal transduction in cells. Using NMR, CD, SPR, etc., we study the three-dimensional structures, conformational changes, dynamics, target binding, and so on. In parallel with these studies, we are also trying computational approaches to predict the structure of protein-protein complexes. The mechanism of biological functions deduced by the physicochemical studies is checked by biochemical experiments. Currently, we are working on a Ca2+ binding protein, calmodulin, and phospho-protein, CPI-17. Both of them are located in smooth muscle. Their functions are shown in Figure 1.



Figure 1. Regulation of smooth muscle contraction. Small circles colored red indicate phosphate groups. MLCK; myosin light-chain kinase, MP; myosin phosphatase, and PKC; protein kinase C.