Poster Presentation

MS98.P01

Observation of electron transfer associated with enzymatic process by muSR

<u>T. Kiyotani¹</u>, M. Kobayashi², I. Tanaka^{3,4}, N. Niimura⁴

¹Showa Pharmaceutical University, Machida, Tokyo, Japan, ²Graduate School of Science and Engineering, Ibaraki University, Hitachi, Ibaraki, Japan, ³College of Engineering, Ibaraki University, Hitachi, Ibaraki, Japan, ⁴Frontier Center for Applied Atomic Sciences, Ibaraki University, Tokai, Ibaraki,

Japan

We propose muSR experiments on trypsin-BPTI complex to visualize the electron and proton transfer processes occurring in the catalytic reaction of the trypsin. The mechanism of an inhibitory effect of the BPTI is interpreted that the reaction products of BPTI remain at a part of the structure and the reverse reaction reforms the stable trypsin–BPTI complex, which has been confirmed by neutron diffraction experiment of the trypsin-BPTI complex [1]. However, it never sees the real image of the proton and electron transfer processes directly. According to the model provided by the results of neutron diffraction experiments, the proton and electron transfer processes are continuously occurring in a crystal of trypsin-BPTI complex and the process induces the local magnetic field. The slow muon is very adequate because the position, where mu+ is captured, is absolutely negatively charged oxyanion hole close to the reaction center of Trypsin. The distance between the oxyanion hole and the active peptide bond is about 10Å. When the turn over time of the catalytic reactions is assumed to be 10msec or so, the induced magnetic field would be estimated as 0.2 micro-T. In order to check the effectiveness of the measurement of the µSR experiments on trypsin-BPTI complex, another measurement of the muSR experiments on the trypsin- MIP complex is adequate [2]. Here, MIP is a kind of the trypsin inhibitor, which completely stops the catalytic reaction of trypsin. In the trypsin-MIP complex, no electron and proton transfers at all in the active site of trypsin and captured mu+ at the oxyanion hole would never be sensitive to the induced magnetic field [3].

[1] K.Kawamura, T.Yamada, K.Kurihara, T.Tamada, R.Kuroki, I.Tanaka, H.Takahashi, N. Niimura, Acta Cryst, 2011, D67, 140-148, [2] A.A. Kossiakoff, Basic Life Sci, 1984, 27, 281-304, [3] N. Niimura, I. Tanaka, M. Kobayashi, JPS Conference Proceedings, 2014, in press.

Keywords: ultra slow muon, electron and proton transfer, catalytic reaction of the trypsin