## $^2$ H- $^{13}$ C 二重標識体を用いた固体 NMR による飽和リン脂質 sn-1、sn-2 アシル鎖 の配座配向解析

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*Sn*-1 and *sn*-2 specific conformation and orientation of phospholipid chains based on solid-state NMR of <sup>2</sup>H-<sup>13</sup>C double labeled acyl segments

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Phospholipids are the major component of cell membranes, and their acyl chains play an important role in the physical properties of the membranes. Although model membrane systems have extensively been investigated so far, the detailed molecular behavior of its hydrocarbon chains involved in raft formation remains unclear. In particular, the orientation of the two acyl chains at the *sn*-1 and *sn*-2 positions has not been proven experimentally. In order to evaluate the difference in conformation and orientation between these acyl chains of DPPC, we synthesized the isotope-labeled lipids in which the acyl chains are site-selectively labeled with deuterium and carbon-13. Based on the solid-state NMR of hydrated lipid bilayers, the differences in the orientation and conformation of the *sn*-1 and *sn*-2 acyl chains are to be elucidated.

リン脂質は細胞膜の主要な脂質成分であり、そのアシル鎖は膜の物性に大きく関わっている。細胞膜におけるリン脂質の動的挙動解析は、主に重水素固体 NMR 測定(²H NMR)によって行われてきた。しかし多くの場合、²H NMR により得られる四極子分裂幅の解析は、アシル鎖が膜に垂直方向の平均配向をとることを前提に、標識位置の運動性が議論されており、実際に標識位置のおけるアシル鎖の配向を求めた例はほとんどない。特にリン脂質が有する二つのアシル鎖(sn-1 位と sn-2 位)の配座配向の違いについては、分子動力学シミュレーションで示唆されているものの実験的には未だ証明されていない。そこで本研究ではモデル脂質として用いられることの多い飽和リン脂質である DPPC(図 1)のアシル鎖の配座・配向について、sn-1 位と sn-2 位の違いを評価することとした。二つのアシル鎖において配座配向の違いが大きいことが示唆されている 9 位、10 位及び 11 位について重水素および炭素13 で位置選択的に標識した 10'-<sup>13</sup>C-9'-d<sub>1</sub>-DPPC、10"-<sup>13</sup>C-9"-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>C-10'-d<sub>1</sub>-DPPC、11'-<sup>13</sup>

図1DPPCの構造