

Product Data Sheet

Product Name: 1,2-Dimyristoyl-rac-glycero-3-phosphocholine

Cat. No.: GA20356

Chemical Properties

Cas. No. 18656-38-7

Formula $C_{36}H_{72}NO_8P$

M.Wt 677.94

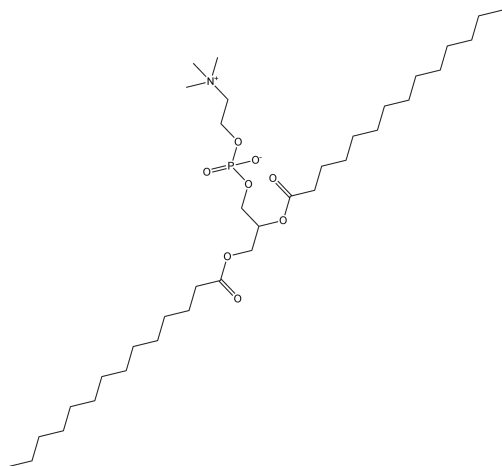
Solubility Soluble in DMSO

Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Protocol

This plan only provides a guide, please modify it to meet your specific needs.

Preparation of 1,2-Dimyristoyl-rac-glycero-3-phosphocholine vesicles^[1]:

- Initially, the required amount of 1,2-Dimyristoyl-rac-glycero-3-phosphocholine lipid (~2mg) was taken in the round-bottom flask and solubilized in a 1:1 chloroform/methanol mixture.
- Subsequently, the mixture was slowly evaporated using a rotary evaporator to produce the thin film of dry lipid at the bottom of the flask.
- The thin film was then hydrated using the required amount of water or DMSO/water mixtures prepared previously, and the volume was adjusted to achieve a final lipid concentration of ~3mM.
- For the spectroscopic studies, sonicate the vesicle solutions by means of an ultrasonic probe.

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sonicator using a pulse of $\sim 20 \pm 3\text{kHz}$, followed by passing the vesicle solution through a 450nm pore size cellulose filter to obtain the uniform distribution of vesicles $\sim 100 \pm 20\text{nm}$ in size.

5. Then the solutions were added to the methanol-evaporated Coumarin 153 (C153) or 4-(dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4H-pyran (DCM) solution as required.

DMSO treatment of 1,2-Dimyristoyl-rac-glycero-3-phosphocholine^[2]:

1. DMSO is used as a cosolvent, and its concentration is gradually increased from 0% to 25%.

Analysis of water dynamics in 1,2-Dimyristoyl-rac-glycero-3-phosphocholine after DMSO treatment^[2]:

1. Lipids are modeled using the Slipid force field, water with the TIP4P/2005 model, and DMSO parameters are derived from General Amber Force Field.

2. PACKMOL is used to arrange lipids, water, and DMSO evenly within the bilayer.

3. Energy minimization is performed using the steepest-descent algorithm.

4. Simulations are conducted in the NPT ensemble with a temperature of 350K and a pressure of 1bar.

5. The bilayer is equilibrated for 800–1000ns with all-bond constraints, followed by 1 μs of NPT simulation without bond constraints.

6. Bilayer properties such as area per lipid, density profile, and thickness are analyzed from the NPT production runs.

References:

[1] Kundu S, Malik S, Ghosh M, et al. A Comparative Study on DMSO-Induced Modulation of the Structural and Dynamical Properties of Model Bilayer Membranes. *Langmuir*. 2021;37(6):2065-2078.

[2] Sahu S, Garg A, Saini R, Debnath A. Interface Water Assists in Dimethyl Sulfoxide Crossing and Poration in Model Bilayer. *Langmuir*. 2024;40(11):5764-5775.

Background

1,2-Dimyristoyl-rac-glycero-3-phosphocholine, a zwitterionic phospholipid, was chosen as a simple but suitable membrane model of the human cell membrane for mimicking the neutral charge of the surface membrane of eukaryotic plasma membranes^[1]. The effect of antibiotics such as Rifabutin on human cell membrane models was assessed using multilamellar vesicles (MLVs) composed of 1,2-Dimyristoyl-rac-glycero-3-phosphocholine^[1-2]. 1,2-Dimyristoyl-rac-glycero-3-phosphocholine can serve as a model lipid membrane to study the effects of DMSO and drugs on eukaryotic cell membranes^[3-5]. 1,2-Dimyristoyl-rac-glycero-3-phosphocholine can also be used to prepare

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polydiacetylene (PDA)^[6]. 1,2-Dimyristoyl-rac-glycero-3-phosphocholine experiences an increase in headgroup area, enhanced membrane disorder, and increased fluidity due to DMSO, but the bilayer does not disintegrate^[4].

References:

- [1] Pinheiro M, Nunes C, Caio JM, et al. The influence of rifabutin on human and bacterial membrane models: implications for its mechanism of action. *J Phys Chem B*. 2013;117(20):6187-6193.
- [2] Pinheiro M, Nunes C, Caio JM, Moiteiro C, Brezesinski G, Reis S. Interactions of N'-acetyl-rifabutin and N'-butanoyl-rifabutin with lipid bilayers: a synchrotron X-ray study. *Int J Pharm*. 2013;453(2):560-568.
- [3] Kundu S, Malik S, Ghosh M, et al. A Comparative Study on DMSO-Induced Modulation of the Structural and Dynamical Properties of Model Bilayer Membranes. *Langmuir*. 2021;37(6):2065-2078.
- [4] Sahu S, Garg A, Saini R, Debnath A. Interface Water Assists in Dimethyl Sulfoxide Crossing and Poration in Model Bilayer. *Langmuir*. 2024;40(11):5764-5775.
- [5] Pinheiro M, Amenitsch H, Reis S. Antituberculosis Drug Interactions with Membranes: A Biophysical Approach Applied to Bedaquiline. *Membranes (Basel)*. 2019;9(11):141.
- [6] Jung YK, Park HG. Colorimetric detection of clinical DNA samples using an intercalator-conjugated polydiacetylene sensor. *Biosens Bioelectron*. 2015;72:127-132.

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