Experimental report

08/01/2021

Proposal: 9-13-840 **Council:** 4/2019

Title: Neutron Reflection Studies on Adsorption of Acyl-L-carnitine at the water/air Interface and its interaction with DPPG monolayer

Research area: Biology

This proposal is a new proposal

Main proposer: Jian Ren LU

Experimental team: Zongyi LI
Lin ZHANG
Huayang LIU
Ke FA
Peter HOLLOWELL

Local contacts: Armando MAESTRO

Samples: DPPG
L-Carnitine
(CH3)3N+-CH2-CHOCO-C14H28-CH2-COO-C14H23
PBS-Buffer(D2O)

Instrument	Requested days	Allocated days	From	To
FIGARO	2	3	04/07/2019	06/07/2019
			17/02/2020	18/02/2020

Abstract:

Acyl L-Carnitines are a group of novel surfactants with attractive physical and biological properties associated with their head group charge features. This work proposes to use neutron reflection as the unique technique to determine how acyl-L-carnitines interact with DPPG monolayer which can help to study how acyl-L-carnitines kill the bacteria. Because the head group has special charge responses to pH, it will be of interest to examine how acyl-L-carnitines interact with DPPG monolayer with pH and ionic strength. We request 2 days of FIGARO beam time to complete the proposed measurements.

Experimental report

03/2020

Proposal: 9-13-840

Council:

Title: Neutron Reflection Studies on Adsorption of Acyl-L-carnitine at the water/air Interface and its interaction with DPPG monolayer

Research area: Biosurfactants,

Main proposer: **Jian Ren LU**

Experimental team: Huayang LIU

Zongyi LI

Ke FA

Local contacts: Armando MAESTRO

Samples: Acyl-L-carnitines

Instrument	Requested days	Allocated days	From	To
FIGARO	2	3	04/07/2019	06/07/2019
			17/02/2020	18/02/2020

Abstract:

Acyl L-Carnitines are a group of novel surfactants with attractive physical and biological properties associated with their head group charge features. This work proposes to use neutron reflection as the unique technique to determine how acyl-L-carnitines interact with DPPG monolayer which can help to study how acyl-L-carnitines kill the bacteria. Because the head group has special charge responses to pH, it will be of interest to examine how acyl-L-carnitines interact with DPPG monolayer with pH and ionic strength. We request 2 days of FIGARO beam time to complete the proposed measurements.

Report of experiment – FIGARO 9-13-840

PhD Project: Study the fundamental properties of acyl-L-carnitines

Huayang LIU

The purpose of this experiment is to study the adsorption of acyl-L-carnitines in water under different concentrations, pH and ionic strength. We use the FIGARO to measure the different contrasts and fit them to have the structural details of adsorbed acyl-L-carnitines layers.

Materials / samples:

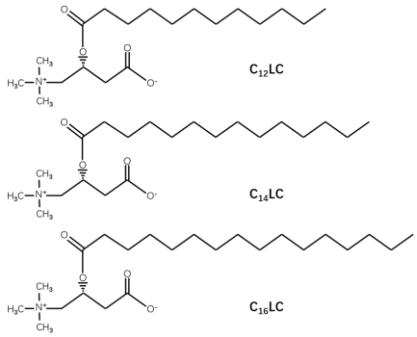

Figure 1 Chemical structure of acyl-L-carnitines

The structure of acyl-L-carnitines are shown in Figure 1. The surfactants have been purified by crystallization method to remove acid and salt, so that the samples have very high purity. The sample powder is dissolved in water with different concentrations, and the pH is adjusted with HCL solution. Then NaCl solution is added to control the ionic strength. Besides, three contrasts are measured in this experiment: h-acyl-L-carnitines are dissolved in D_2O, d-acyl-L-carnitines are dissolved in null reflection water(NRW) and D_2O. The ready samples are poured into the Teflon troughs and measured at 25℃.

Experiment and results

Firstly, 2mM $C_{12}LC$, 0.2mM $C_{14}LC$ and 0.02mM $C_{16}LC$ were measured with 3 contrasts at 25℃. H sample in D_2O was measured for 45mins, D sample in NRW was measured for 30min and D sample in D_2O was measured for 45mins. Then $dC_{12}LC$ (0.6mM and 0.2mM), $dC_{14}LC$ (0.06mM and 0.02mM) and $dC_{16}LC$ (0.006mM and 0.002mM) in NRW were measured.

Figure 2 shows the NR data profiles for $C_{12}LC$. In Figure (a), the red is $hC_{12}LC$(2mM) in D_2O and multiplying 10 times to give a clear view. The green is $dC_{12}LC$ in D_2O and The blue is $dC_{12}LC$ in NRW. The SLD values of different parts used in neutron reflection data are shown in Table 1. Table 1 shows that the deuterated acyl chains have a SLD value of 7 and protonated acyl chains have a SLD value of -0.4. Figure 2(b) shows that the reflectivity from adsorbed layer increases as the concentration rises. The best-fitted parameters shows the thickness of $C_{12}LC$, $C_{14}LC$ and $C_{16}LC$ layers are 21 Å, 22 Å and 24 Å, respectively. At pH7, the ionic strength has little effect on the adsorption amount of acyl-L-carnitines on the interface of air/water. When pH decreases to pH2, the thickness of adsorbed layers has a little increment. And from the Figure 2(a), we can get further structure parameters, the layer in the air is about 12 Å and the layer under water is about 9 Å for $C_{12}LC$.

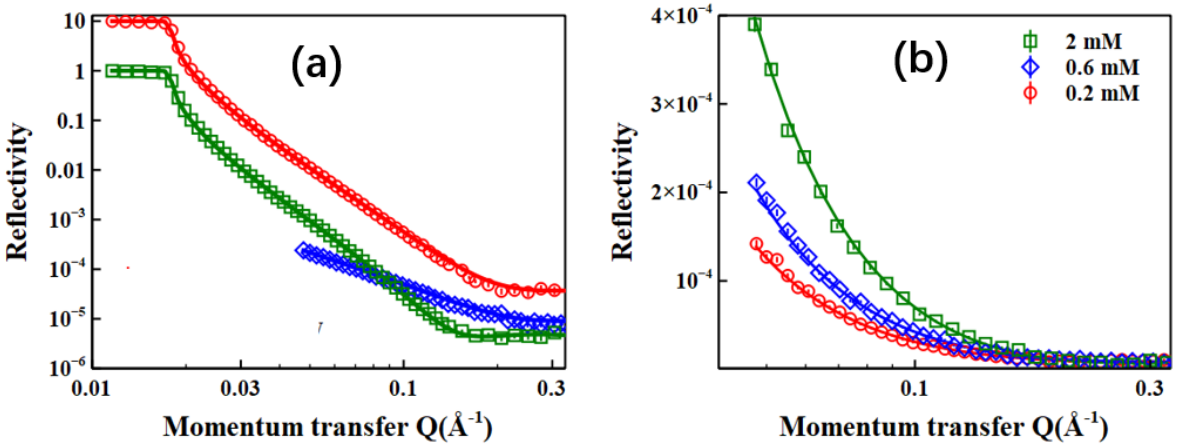

Figure 2 Neutron reflection profiles of $C_{12}LC$ for 3 contrasts at pH7 at 2mM (a), for d-$C_{12}LC$ in NRW with 3 contrasts (b).

Segments	Scattering length density/ρ(Å^{-2}×10^{-6})
Protonanted tail ($C_{11}H_{23}$)	-0.40
Deuterated tail ($C_{11}D_{23}$, 98%D)	7.01
Protonanted tail ($C_{13}H_{27}$)	-0.39
Deuterated tail ($C_{13}D_{27}$, 98%D)	7.03
Protonanted tail ($C_{15}H_{31}$)	-0.37
Deuterated tail ($C_{15}D_{31}$, 98%D)	7.00
Head(hL-carnitine with -C=O)	1.31
Null reflection water(NRW)	0
D_2O	6.35

Table 1 The SLD of different segments used in fitting NR data

Conclusion

The adsorption amount of acyl-L-carnitines on the interface of air/water increase as the concentration increase.

The thickness of acyl-L-carnitine layer increase with the acyl chain length.

Ionic strength has little effect on the structure of layer at pH7.

Low pH environment increase the thickness of layer.