Supporting information for

Tripod facial surfactants with benzene as central core: design, synthesis and self-assembly study

Julien Dauvergne^{*a,b*}, Anissa Bendjeriou^{*a,b*}, Françoise Bonneté^{*a,b*}, Joachim Kolhbrecher^{*c*}, Bernard Pucci^{*a,b*}, Laurie-Anne Barret^{*a,b*} and Ange Polidori^{*a,b*},*

^a Université d'Avignon et des Pays de Vaucluse, Faculté des Sciences, Équipe Chimie Bioorganique et Systèmes Amphiphiles,
33, rue Louis Pasteur, 84000 Avignon, France
Fax: (+33) 04 90 14 44 49, E-mail: <u>ange.polidori@univ-avignon.fr;</u>
^b Institut des Biomolécules Max Mousseron, UMR 5247, CNRS - Universités Montpellier I et II
15, avenue Charles Flahault, 34093 Montpellier cedex 05, France
^c Laboratory for Neutron Scattering
Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Table of contents

Page

1)	¹ H and ¹³ C NMR Spectra scanned	2
2)	Electron microscopy visualisation by negative staining	8
3)	Small Angle X-Ray Scattering data	10

¹H NMR and ¹³C NMR spectra scanned



¹³C NMR (DMSO) for compound C3Glu3.

Electronic Supplementary Material (ESI) for New Journal of Chemistry This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2012



¹³C NMR (DMSO) for compound C4Glu3.



¹H NMR (DMSO) for compound **C5Glu3**.



Electronic Supplementary Material (ESI) for New Journal of Chemistry This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2012



Electronic Supplementary Material (ESI) for New Journal of Chemistry This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2012



¹³C NMR (DMSO) for compound C7Glu3.

7









Electron microscopy visualisation by negative staining

A solution of the compound **C7Glu3** at 10 mg/mL was sonicated with a microprobe during 15 min and/or 1 h in a bath at 50°C to allow the formation of vesicles. The solutions were passed through a 0.45 μ m filter. A drop of the sample was layed down on a metallic grid coated with a film of carbon and the excess of liquid was imbibed with a blotting paper. Then, a drop of a 3% ammonium molybdate was put on the grid. We waited 30 s to optimise the adsorption and the excess of liquid was removed again. The visualisation by electron microscopy with negative coloration was monitored on a Philips CM/2 transmission electron microscope.



Figure 1. Pictures of compound C7Glu3.

The same sonicated samples was analysed by DLS. These results were collected in the table below and compared to particle sizes found by TEM.

Table 1. Data of vesicles for compound C7Glu3 measured by DLS.

Compound	d (nm) DLS	% (volume)	d ½ (nm)	Count rate (kcps)	d (nm) MET ^a
C7Glu3	538.0	52%	149.7	269.7	167-233

^a Values correspond to the interval between the smaller and the bigger particles observed on the pictures.

Table 2 SAXS data of CnGlu3 ($n=3, 4, 5$) vs. concentration (g.L ⁻¹):								
Entry	c (g/L)	MW [#] (g/mol)	Rg § (nm)	H¶(nm)	Nagg			
C3Glu3	2.4 44	941.2 3003.4	1.18 1.40	n a n a	0.8 2.7			
C4Glu3	2.6* 42	2480.8 8280.0	1.56 1.93	n a 5.8	2.1* 7.1			
C5Glu3	2.8 5.6 11.2 22.5 42	16244 19355 24995 32452 45513	3.61 3.76 4.19 4.85 5.67	6.4 7.9 10.5 14	13 16 20 27 38			

[#] Molecular mass calculated from forward intensity; [§] Radius of gyration obtained from Guinier approximation; [¶] Height of rod obtained from SASfit models

* This value is an intermediate state between the monomer, which could be characterized at CMC or below, and the final aggregate. Measurement below CMC could not be done because of a poor SAXS signal below the CMC or CAC.





10



Figure 2. SAXS patterns of C3Glu3 (A) C4Glu3 (B) and C5Glu3 (C) as a function of concentration. Guinier plots are shown in insert.

Electronic Supplementary Material (ESI) for New Journal of Chemistry This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2012



Figure 3. Pair distribution function of C5Glu3 at different concentrations