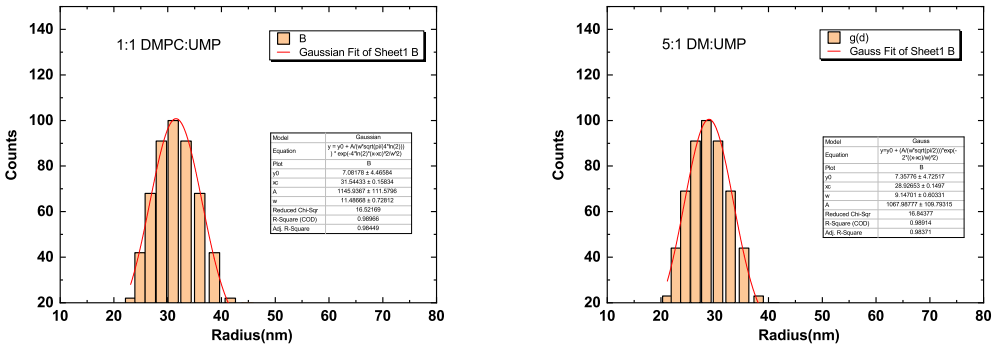
Supporting Information

1 Dynamic light scatterring measurements on DMPC:UMP samples

Size distribution of vesicles formed in DMPC:UMP samples was determined using DLS. Samples were equilibrated at 60°C before the measurement. Figures 1 (a) and (b) show the distribution of vesicle radius in the 1:1 and 5:1 samples, respectively. The average radius in both cases is around 30 nm.



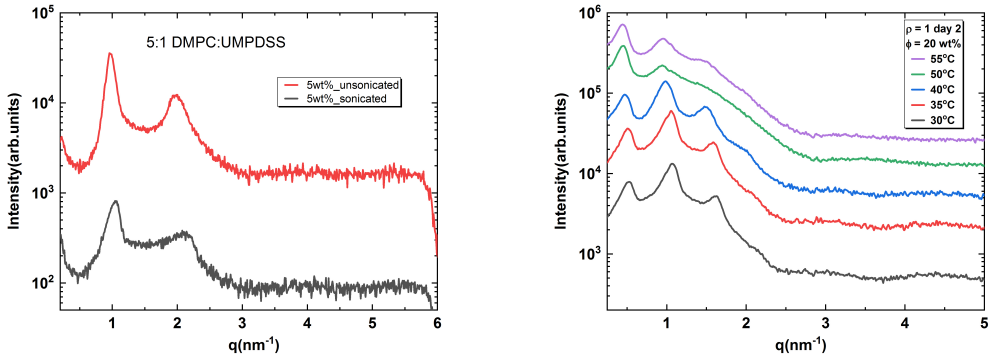
(a) (b)

Figure 1: Distribution of vesicle radius in (a)1:1 and (b) 5:1 DMPC-UMP samples measured by DLS.

2 Small angle x-ray scattering

SAXS measurements were carried out on freshly sonicated and unsonicated DMPC:UMPDSS samples of molar ratio 5:1 (Figure 2(a)). Both samples were very turbid in appearance. SAXS data are consistent with a lamellar phase of periodicity 6.43 nm, which is 0.3 nm higher than that of pure DMPC. Sonication is found to lead to a significant contribution from uncorrelated bilayers to the SAXS data, indicating the formation of ULVs. Nevertheless sonication for 20 minutes was not sufficient to completely disrupts the MLVs in the solution.

SAXS data from a 1:1 DMPC:UMP sample at a lipid concentration of 20 wt% is shown in Figure 2 (b) for a few temperatures. The patterns show the presence of a highly swollen lamellar phase having a periodicity of about 12 nm. The presence of more than 3 peaks in the patterns is consistent with an electrostatically stabilized lamellar phase.



(a) (b)

Figure 2: (a) SAXS data from freshly sonicated and unsonicated 5:1 DMPC-UMP samples. Note the broad background in the case of sonicated sample arising from ULVs. (b) SAXS data from a 1:1 DMPC-UMP sample at a lipid concentration of 20 wt%, showing the presence of a highly swollen lamellar phase.

3 UMP force field

The UMP molecule was added to the force field (in merged.rtp) based on the force field entry of uracil. A hydrogen (H3T) and an oxygen (O3P) were added to form the UMP molecule. The atom type of O3P corresponds to the other oxygen atoms bound to the phosphorus atom in phosphate groups and the atom type of the H3T corresponds to the hydrogen atom on the other hydroxyl group on the sugar ring. Partial charges for the sugar ring and the phosphate group were based on that of AMP. Additionally, an ump.itp file was built to be included in the topology file. The content of ump.itp can be seen below:

```
[ moleculetype ]
; Name            nrexcl
Other               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB      massB
; residue   1 UMP rtp UMP  q -2.0
     1          P      1    UMP      P      1        1.1     30.974   ; qtot 1.1
     2        ON3      1    UMP    O1P      2       -0.9    15.9994   ; qtot 0.2
     3        ON3      1    UMP    O2P      3       -0.9    15.9994   ; qtot -0.7
     4        ON3      1    UMP    O3P      4       -0.9    15.9994   ; qtot -1.6
     5        ON2      1    UMP    O5'      5      -0.18    15.9994   ; qtot -1.78
     6       CN8B      1    UMP    C5'      6       0.09     12.011   ; qtot -1.69
     7        HN8      1    UMP    H5'      7       0.09      1.008   ; qtot -1.6
     8        HN8      1    UMP   H5''      8       -0.4      1.008   ; qtot -2
     9        CN7      1    UMP    C4'      9       0.11     12.011   ; qtot -1.89
    10        HN7      1    UMP    H4'     10       0.09      1.008   ; qtot -1.8
    11       ON6B      1    UMP    O4'     11       -0.4    15.9994   ; qtot -2.2
    12       CN7B      1    UMP    C1'     12       0.11     12.011   ; qtot -2.09
    13        HN7      1    UMP    H1'     13       0.09      1.008   ; qtot -2
    14       NN2B      1    UMP     N1     14      -0.34     14.007   ; qtot -2.34
    15        CN3      1    UMP     C6     15        0.2     12.011   ; qtot -2.14
    16        HN3      1    UMP     H6     16       0.14      1.008   ; qtot -2
    17       CN1T      1    UMP     C2     17       0.55     12.011   ; qtot -1.45
    18        ON1      1    UMP     O2     18      -0.45    15.9994   ; qtot -1.9
    19       NN2U      1    UMP     N3     19      -0.46     14.007   ; qtot -2.36
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    20        HN2      1    UMP     H3     20       0.36      1.008   ; qtot -2
    21        CN1      1    UMP     C4     21       0.53     12.011   ; qtot -1.47
    22        ON1      1    UMP     O4     22      -0.48    15.9994   ; qtot -1.95
    23        CN3      1    UMP     C5     23      -0.15     12.011   ; qtot -2.1
    24        HN3      1    UMP     H5     24        0.1      1.008   ; qtot -2
    25       CN7B      1    UMP    C2'     25       0.14     12.011   ; qtot -1.86
    26        HN7      1    UMP   H2''     26       0.09      1.008   ; qtot -1.77
    27        ON5      1    UMP    O2'     27      -0.65    15.9994   ; qtot -2.42
    28        HN5      1    UMP    H2'     28       0.42      1.008   ; qtot -2
    29        CN7      1    UMP    C3'     29       0.14     12.011   ; qtot -1.86
    30        HN7      1    UMP    H3'     30       0.09      1.008   ; qtot -1.77
    31        ON5      1    UMP    O3'     31      -0.65    15.9994   ; qtot -2.42
    32        HN5      1    UMP    H3T     32       0.42      1.008   ; qtot -2

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[ dihedrals ]
;  ai    aj    ak    al funct            c0            c1            c2            c3
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   21    19    23    22     2

; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif
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