Characterization of 1,2-Distearoyl-*sn*-glycero-3-phosphoethanolamine-*N*-[Methoxy(polyethylene glycerol)-2000] and Its Complex with Doxorubicin Using Nuclear Magnetic Resonance Spectroscopy and Molecular Dynamics

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Running Title: NMR and MD analysis of Dox-DSPE-PEG_{2000}

SUPPLEMENTARY FIGURES

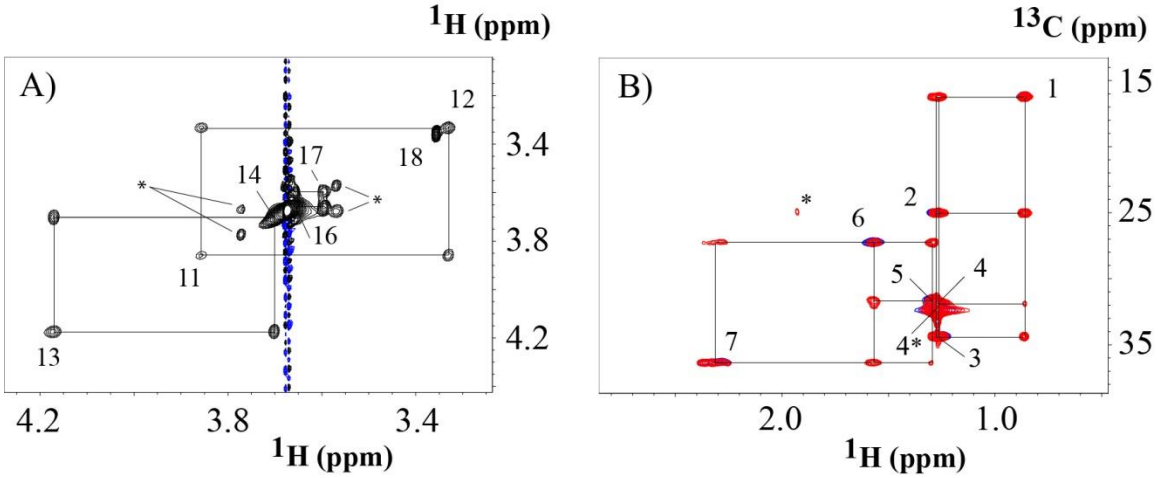

Figure S1. 2D TOCSY, HSQC and HSQC-TOCSY spectra of DSPE-PEG$_{2000}$. (**A**) 2D TOCSY correlations of individual ethylene glycol units at both sides of main body of polyethylene glycol. (**B**) Overlay of HSQC (blue color) and HSQC-TOCSY (red color) spectra from end of fatty acyl chains, and the region close to lipid head groups of DSPE lipid (See Figure 1B for DSPE-PEG$_{2000}$ numbering scheme). The cross peaks denoted with * in A) are from the J coupling between ^{1}H and natural abundance of ^{13}C, and the peak labeled with * in B) is from residual proton of NaAc-d$_3$.

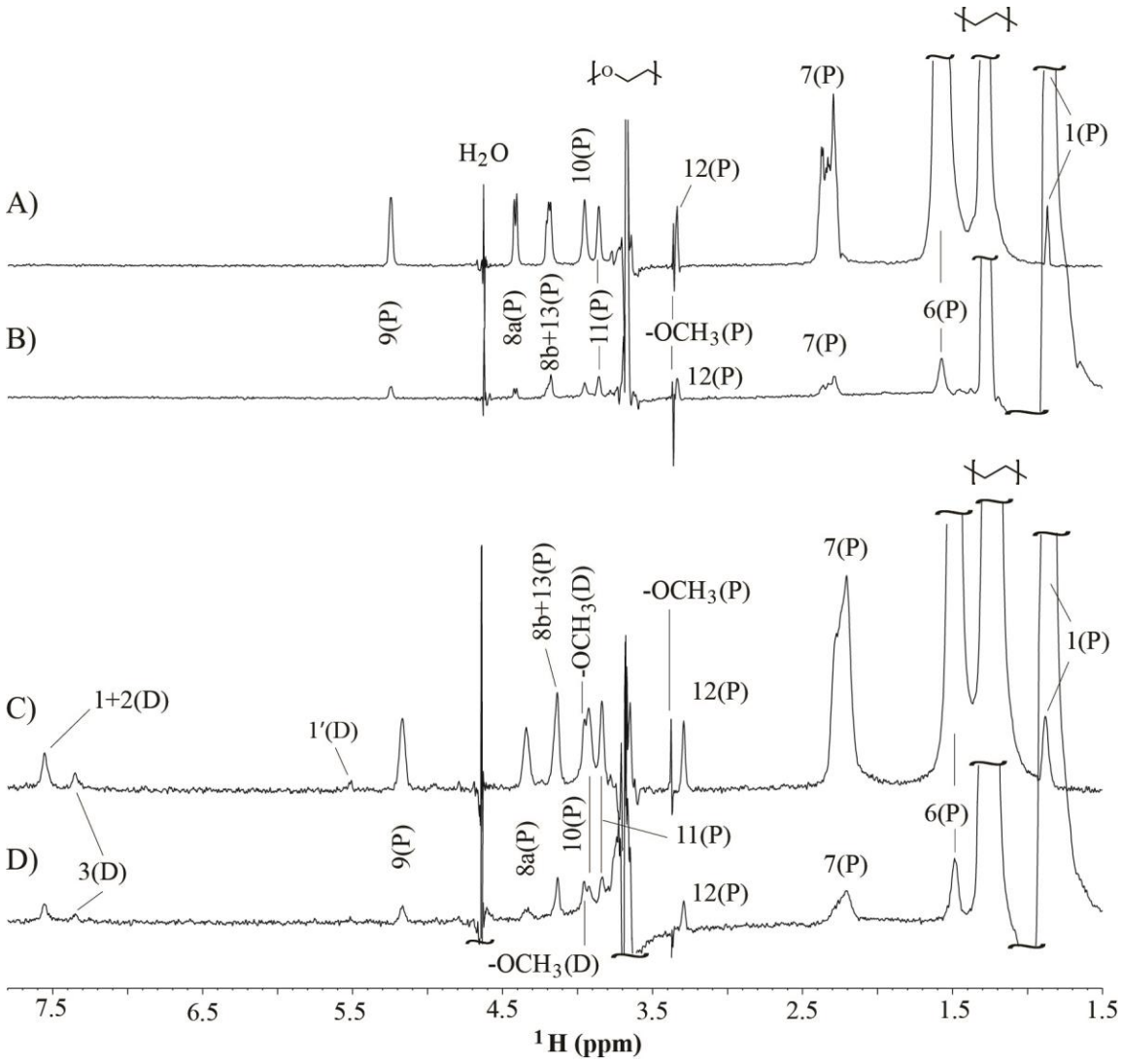

Figure S2. Vector details of the NOESY spectra of the DSPE-PEG$_{2000}$ with and without DOX. (**A**) A 1D slice along the direct dimension taken at position of 6H(P) and (**B**) A 1D slice along the direct dimension taken at position of 1H(P) from 2D NOESY acquired on the free DSPE-PEG$_{2000}$. (**C**) A 1D slice along the direct dimension taken at position of 6H(P) and **D**) 1D slice along the direct dimension taken at position of 1H(P) from 2D NOESY acquired on the complex composed of 3.4 mM Dox and 3.7 mM DSPE-PEG$_{2000}$. There are base line distortions at strong and sharp peaks of -OCH_3(P), H_2O, 15*H(P) and 4*H(P) positions. In order to observe peaks close to strong peaks of 15*H(P) and 4*H(P) clearly, pre-saturation was used simultaneously to suppress these two peaks.