Supporting Information For:

An Efficient Synthesis of γ-Hydroxy-α,β-unsaturated Aldehydic Esters of 2-Lysophosphatidylcholine

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Contents

General methods.

Proton magnetic resonance (^{1}H NMR) spectra and carbon magnetic resonance (^{13}C NMR) spectra were recorded on a Varian Inova AS400 spectrometer operating 400 MHz or 75 MHz. Proton chemical shifts are reported in parts per million (ppm) on δscale relative to $CDCl_3$ (δ 7.26) or CD_3OD (δ 3.31). ^{1}H NMR spectral data are tabulated in terms of multiplicity of proton absorption (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad), coupling constants (Hz), number of protons. gCOSY experiment was done on a spectrometer at 400 MHz. All high resolution mass spectra were recorded on a Kratos AEI MS25 RFA high resolution mass spectrometer at 20 eV. FT-IR was obtained as KBr pellets using an MIDAC Co. M2000. All solvents were distilled under a nitrogen atmosphere prior to use, and all materials were obtained from Aldrich unless specified. Flash chromatography was performed with ACS grade solvent. R_f values are quoted for TLC plates of thickness 0.25 mm. The plates were visualized with iodine, dinitrophenylhydrazine or phosphomolybdic acid reagents. Flash column chromatograph was performed on 230-400 mesh silica gels supplied by Whatman and Sorbent.

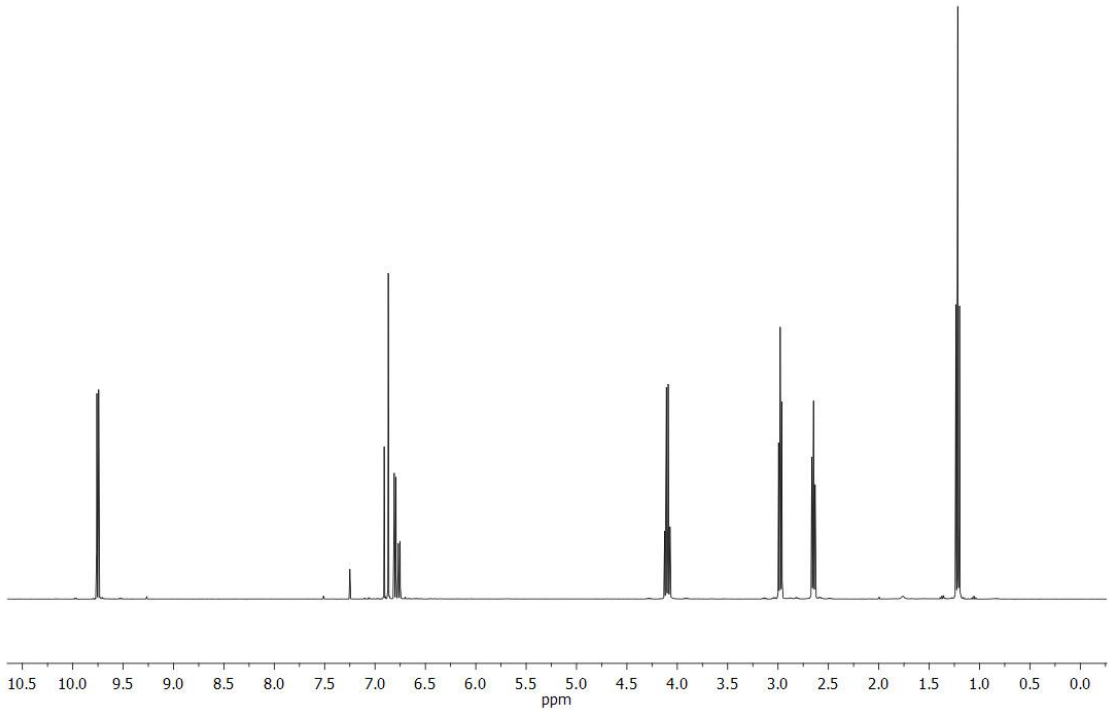

Figure S1 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of Ethyl (*E*)-4,7-dioxohept-5-enoate (**8**)

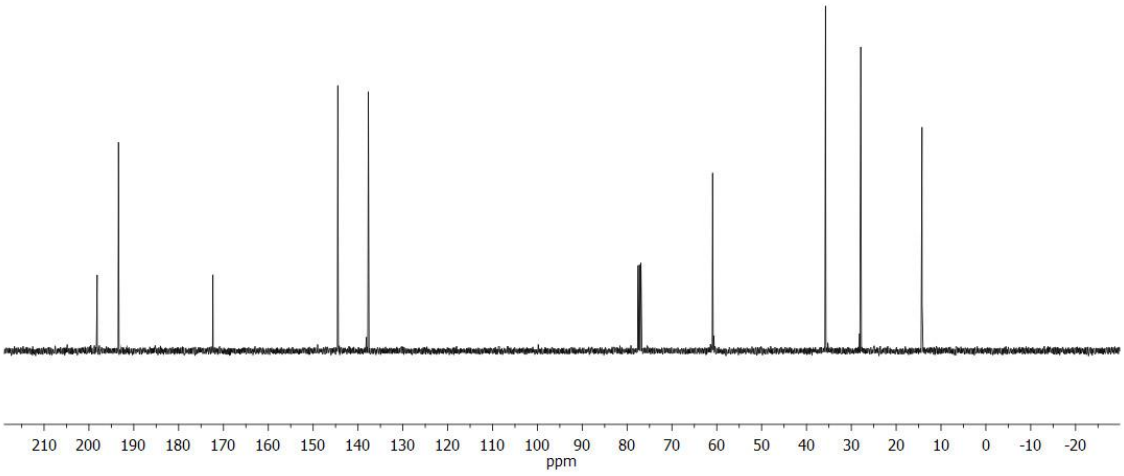

Figure S2 The 100MHz ^{13}C NMR ($CDCl_3$) spectrum of Ethyl (*E*)-4,7-dioxohept-5-enoate (**8**)

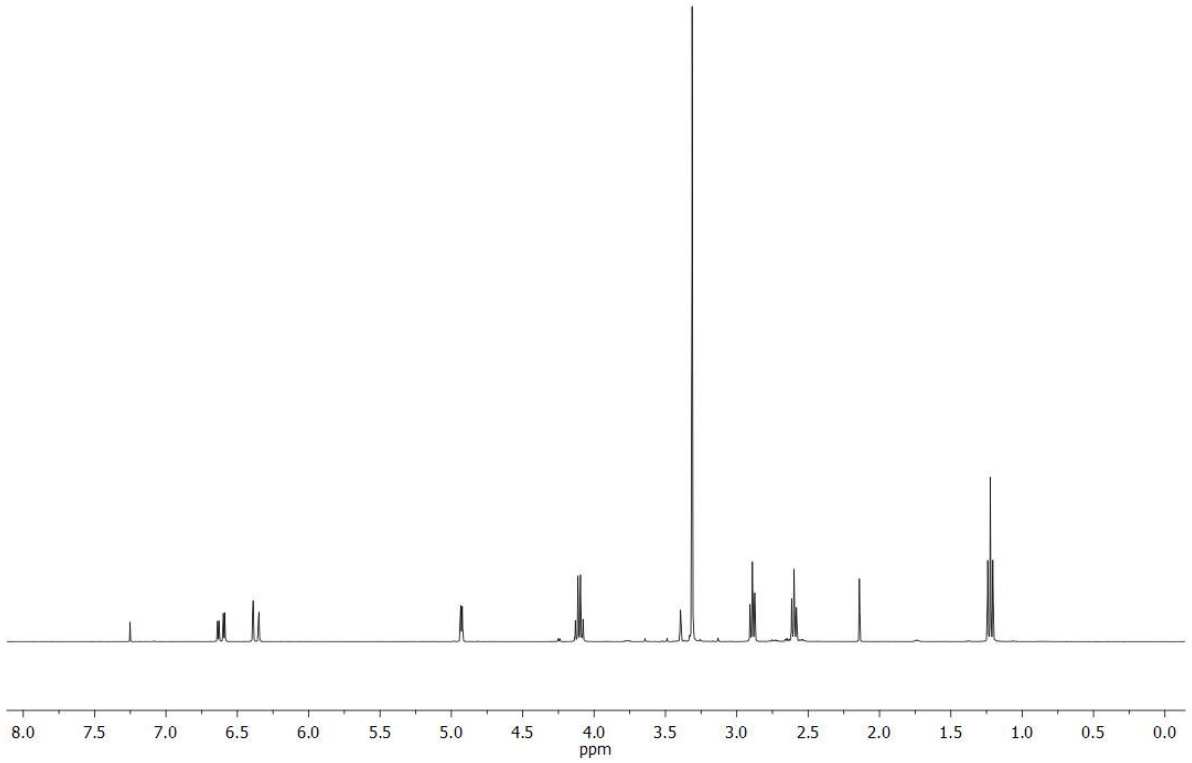

Figure S3 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of Ethyl (*E*)-7,7-dimethoxy-4-oxohept-5-enoate (**9**)

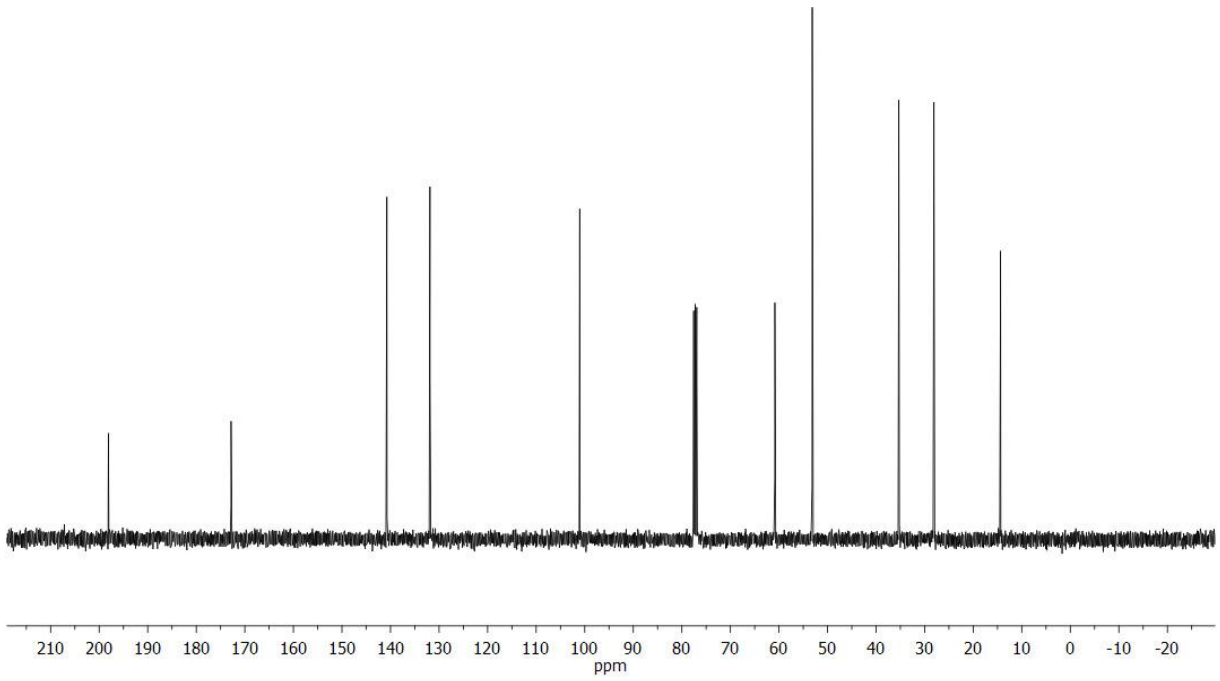

Figure S4 The 100MHz ^{13}C NMR ($CDCl_3$) spectrum of Ethyl (*E*)-7,7-dimethoxy-4-oxohept-5-enoate (**9**)

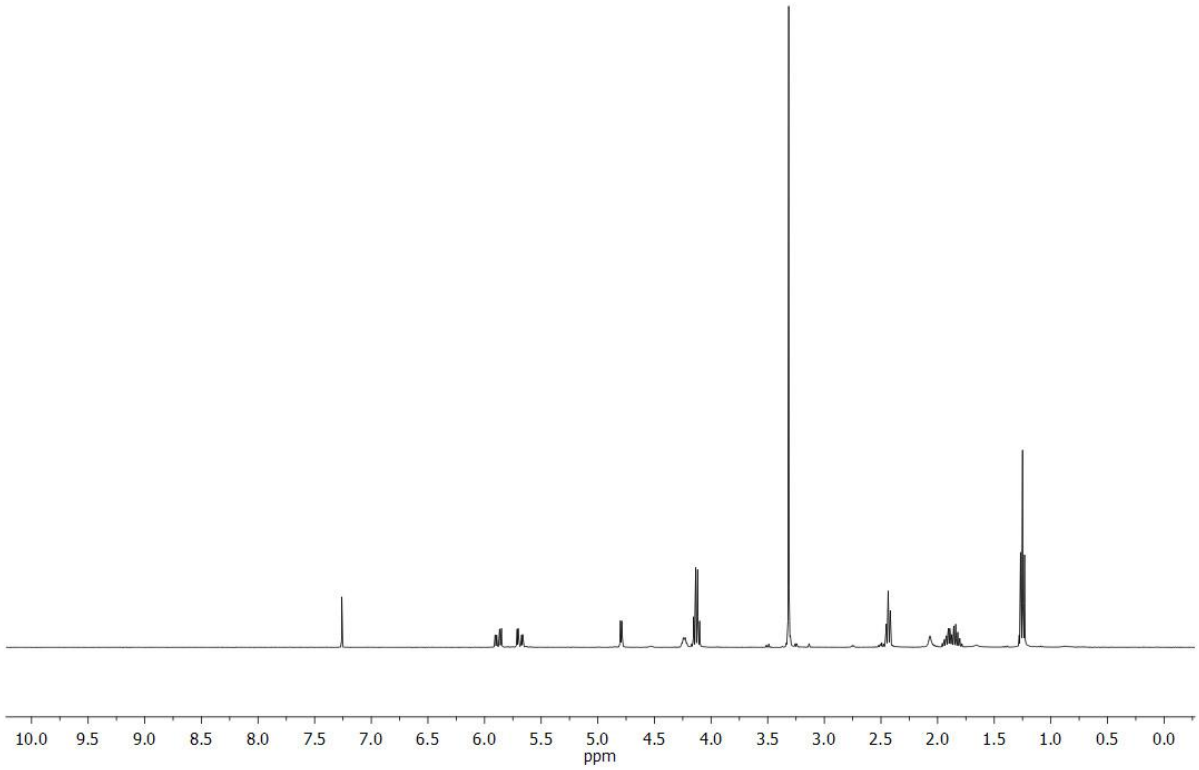

Figure S5 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of Ethyl (*E*)-4-hydroxy-7,7-dimethoxyhept-5-enoate (**10**)

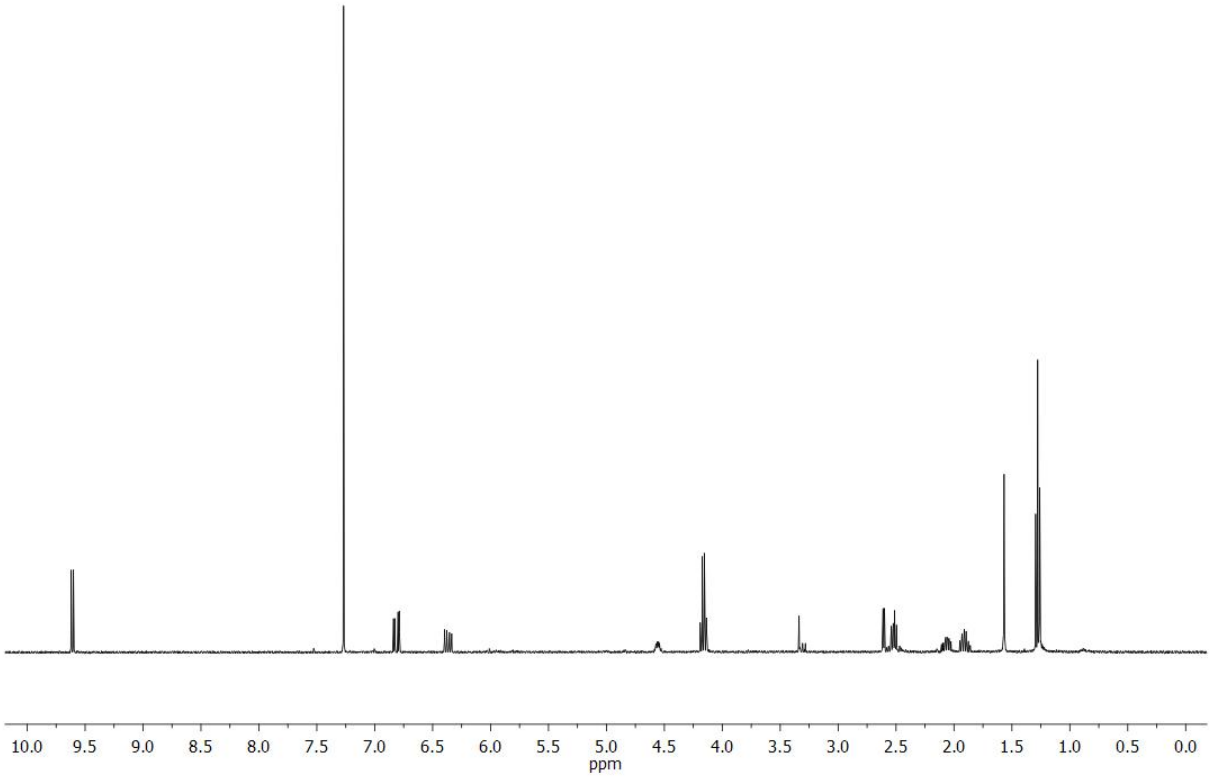

Figure S6 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of Ethyl (*E*)-4-hydroxy-7,7-dimethoxyhept-5-enoate **(11)**

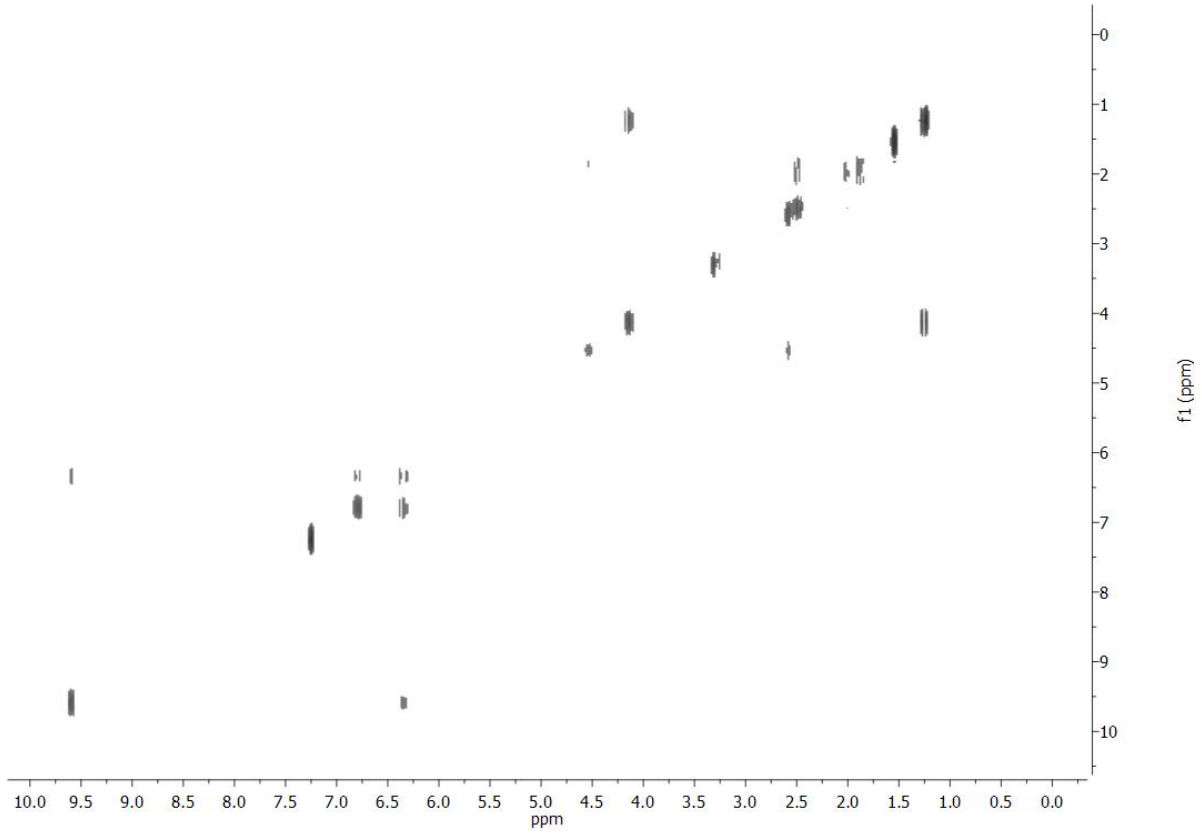

Figure S7 The 400MHz gCOSY NMR ($CDCl_3$) spectrum of Ethyl (*E*)-4-hydroxy-7,7-dimethoxyhept-5-enoate (**11**)

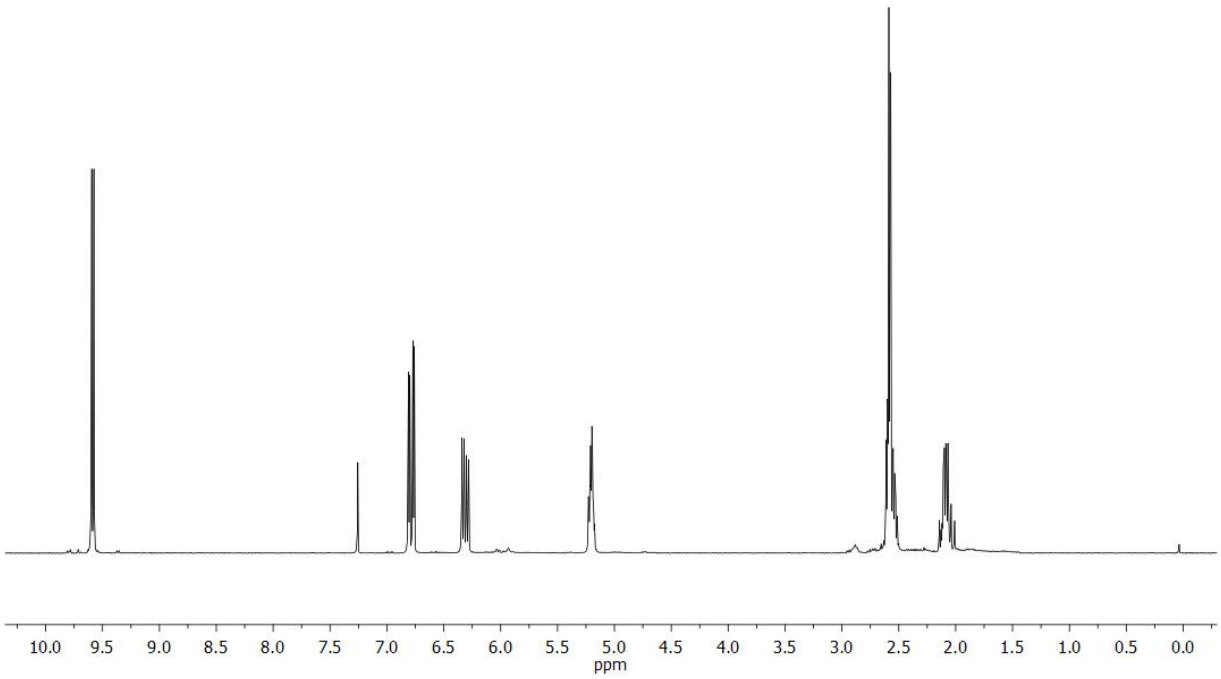

Figure S8 The 400MHz ^1H NMR ($CDCl_3$) spectrum of (*E*)-3-(5-oxotetrahydrofuran-2-yl)acrylaldehyde (**12**)

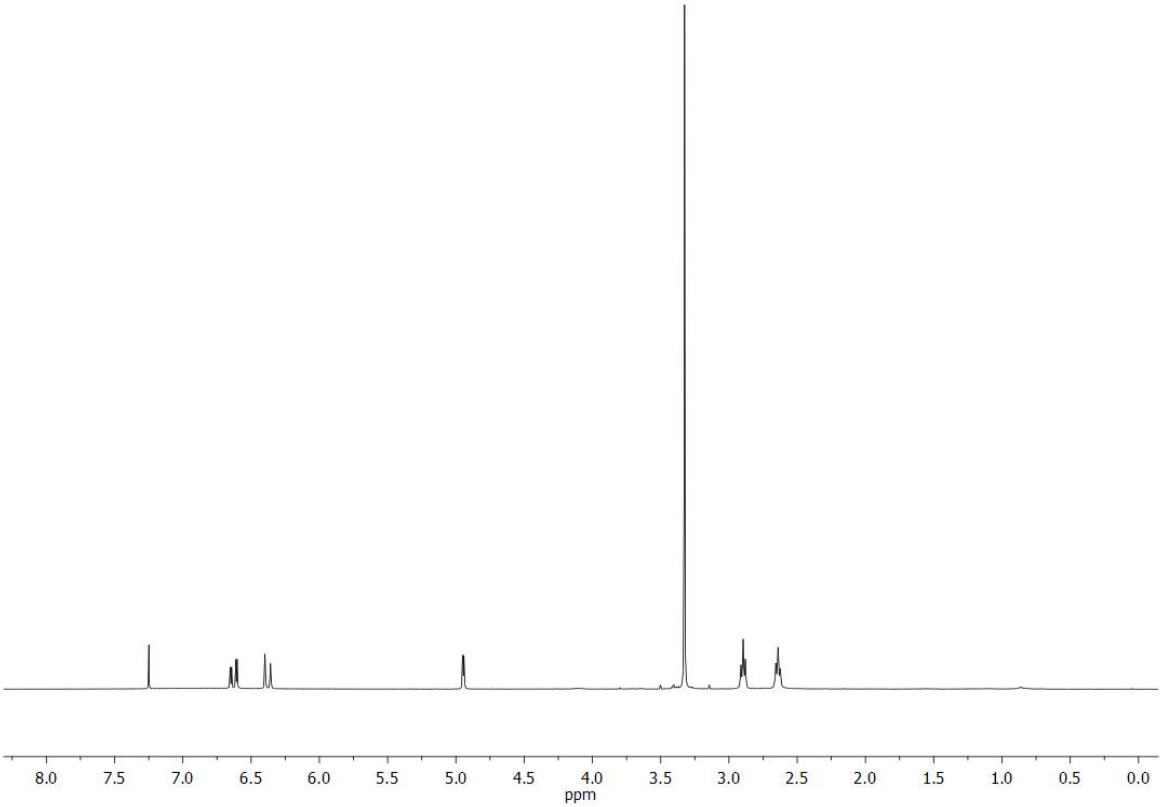

Figure S9 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-7,7-dimethoxy-4-oxohept-5-enoic acid (**3a**)

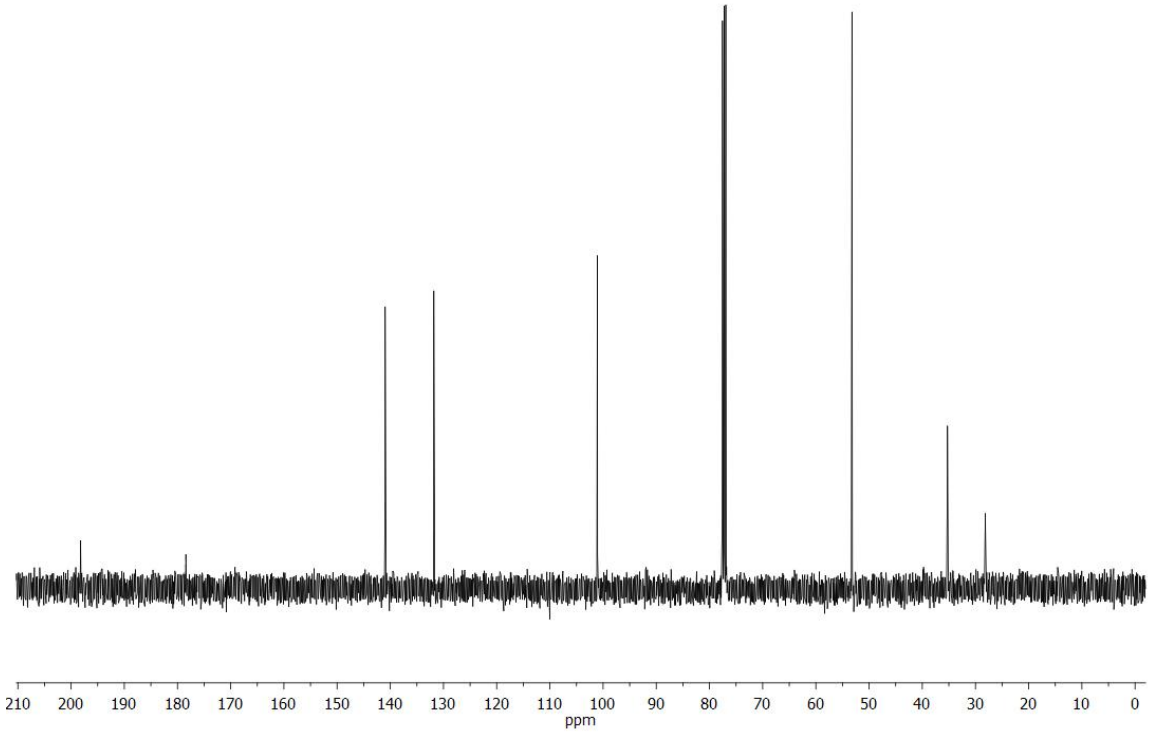

Figure S10 The 100MHz ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-7,7-dimethoxy-4-oxohept-5-enoic acid (**3a**)

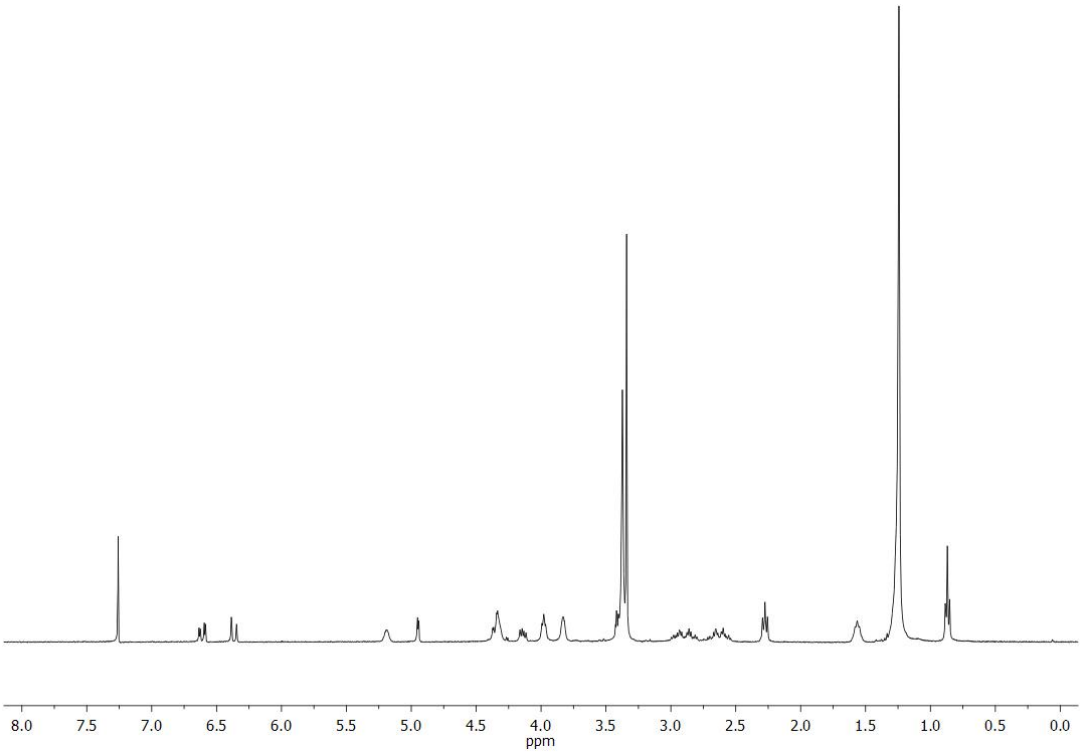

Figure S11 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(7,7-dimethoxy-4-oxohept-5-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**18a**)

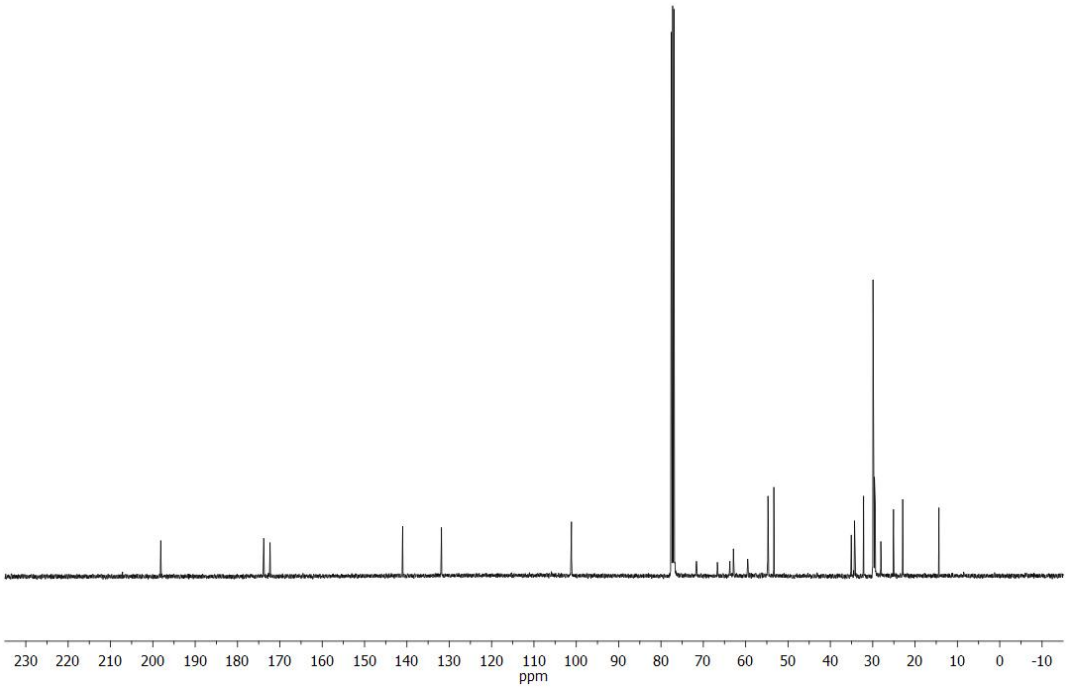

Figure S12 The 100MHz ^{13}C NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(7,7-dimethoxy-4-oxohept-5-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**18a**)

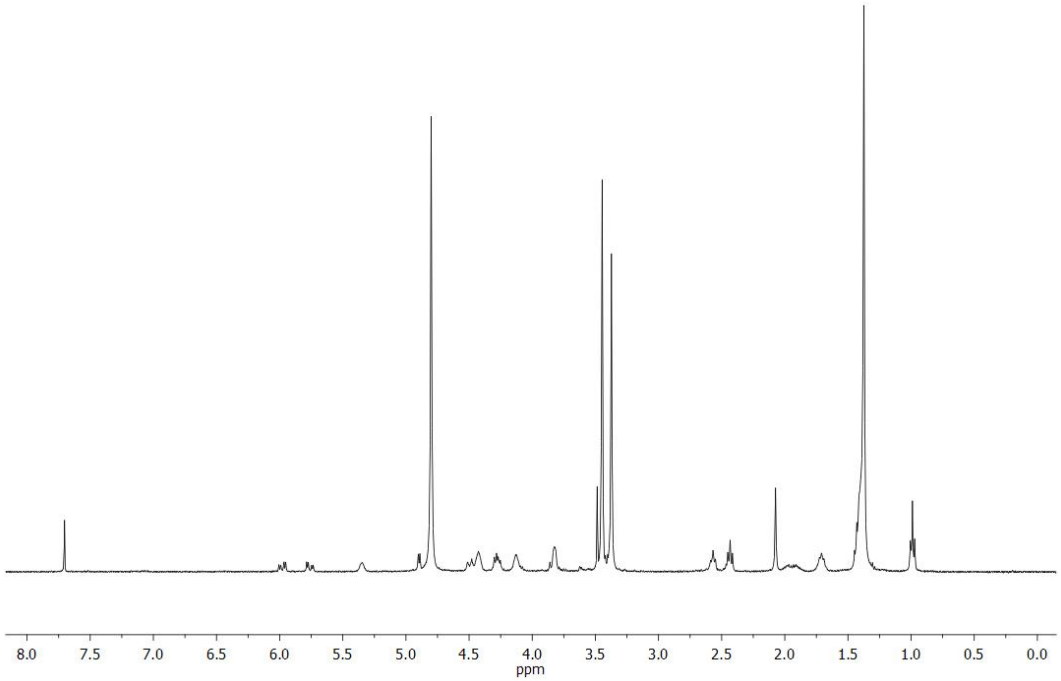

Figure S13 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(4-hydroxy-7,7-dimethoxyhept-5-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**2a**)

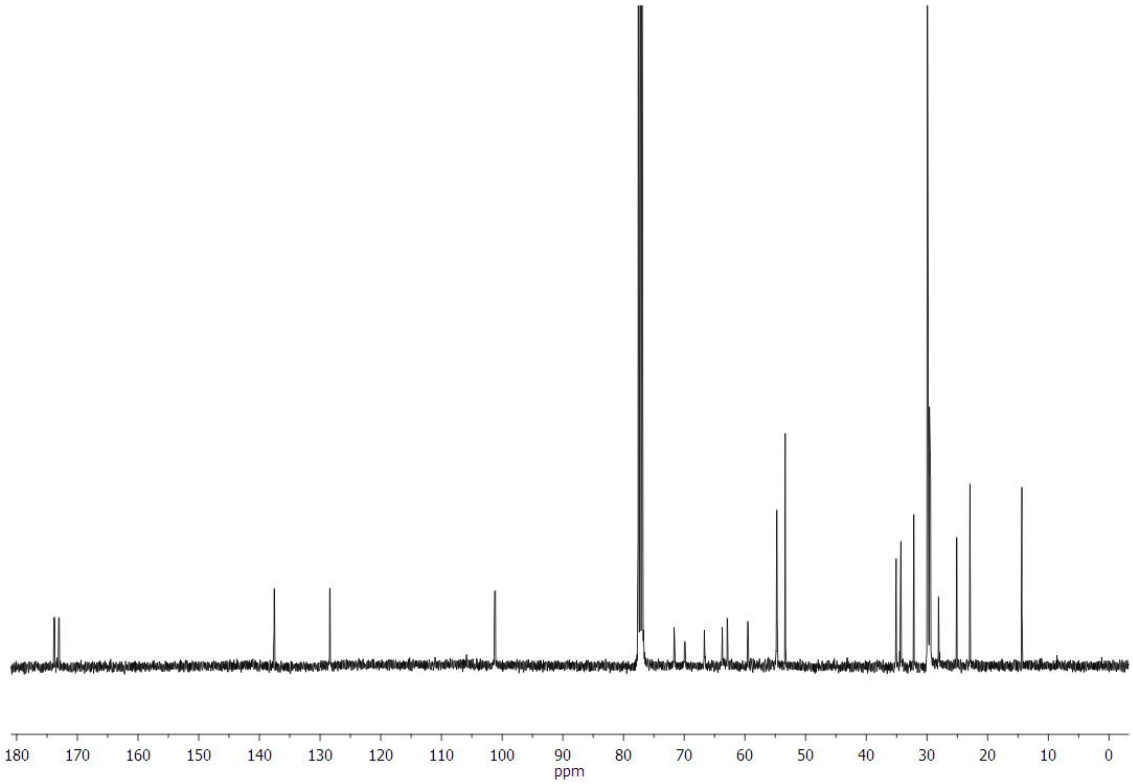

Figure S14 The 100MHz ^{13}C NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(4-hydroxy-7,7-dimethoxyhept-5-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**2a**)

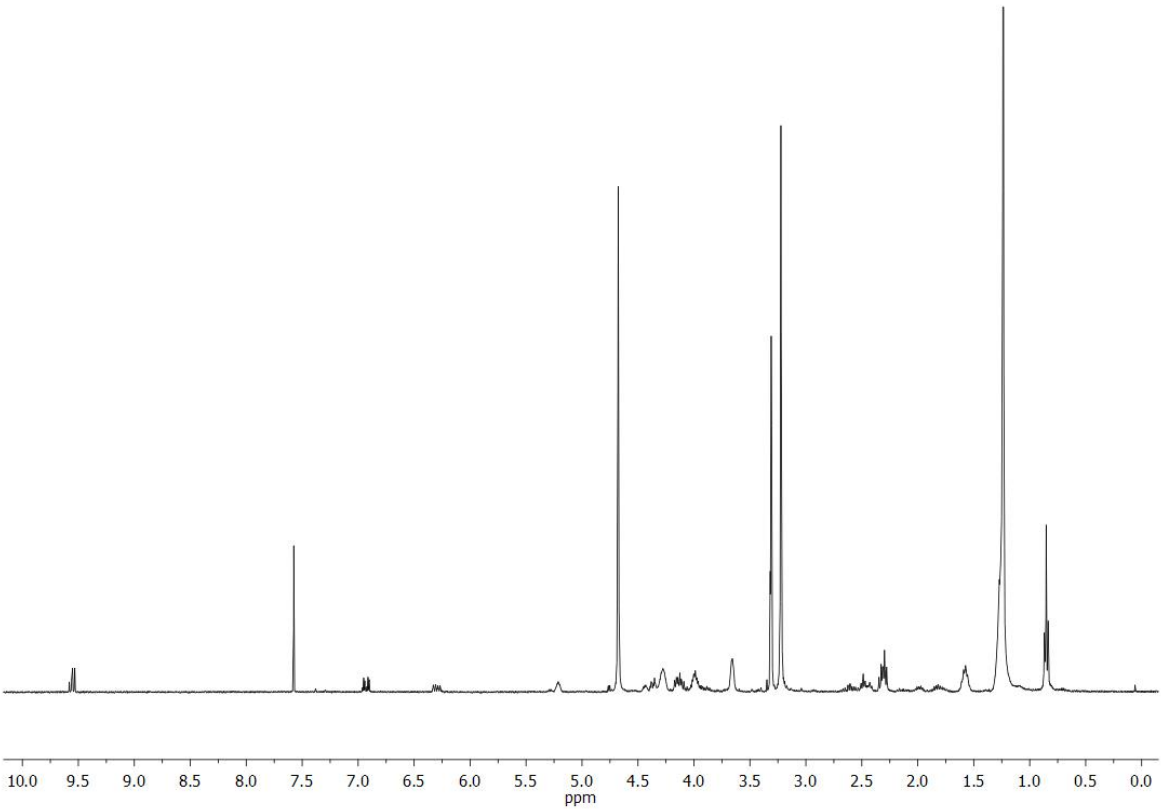

Figure S15 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(4-hydroxy-7-oxohept-5-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**HOHA-PC, 1a**)

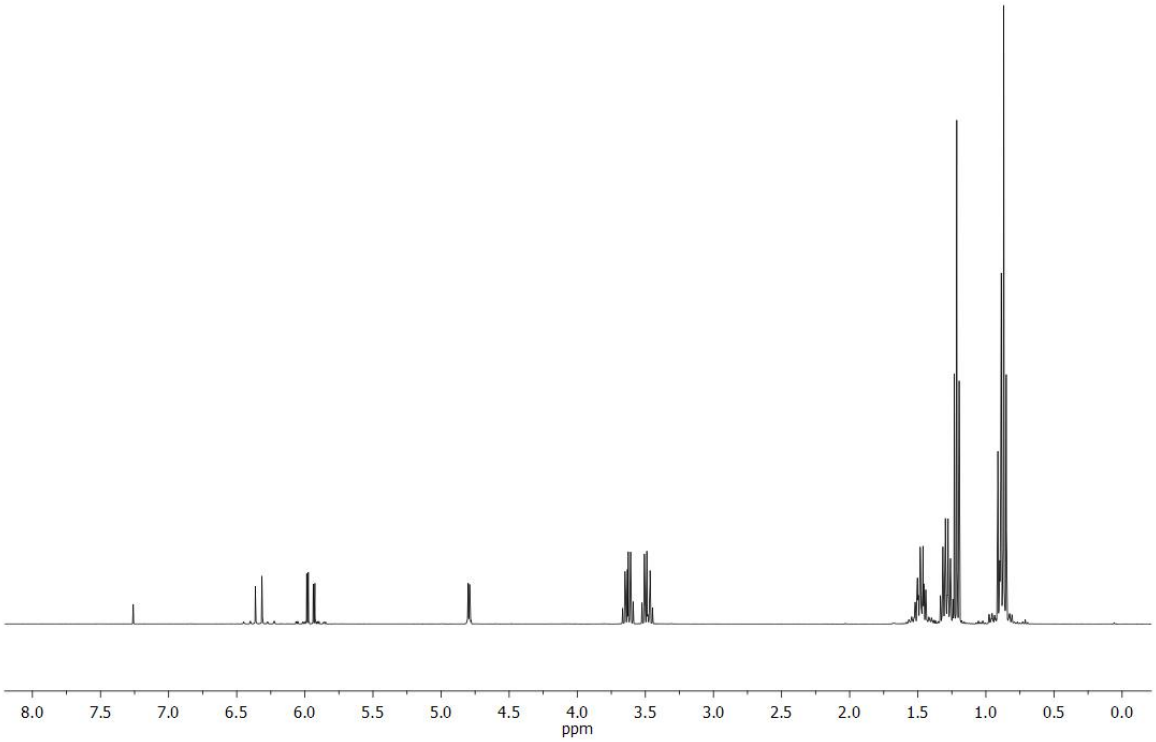

Figure S16 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of 1-tributylstannyl-3,3-diethoxy-prop-1-ene (**4**)

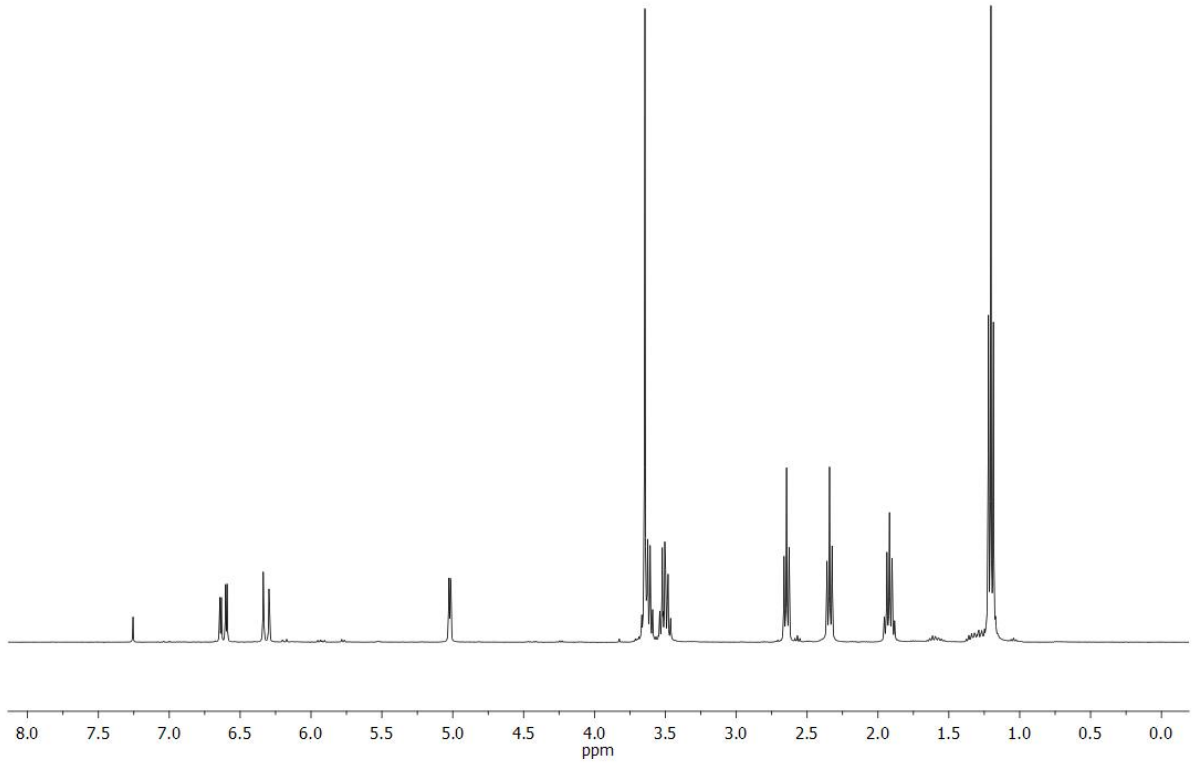

Figure S17 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of Methyl (*E*)-8,8-diethoxy-5-oxooct-6-enoate (**14b**)

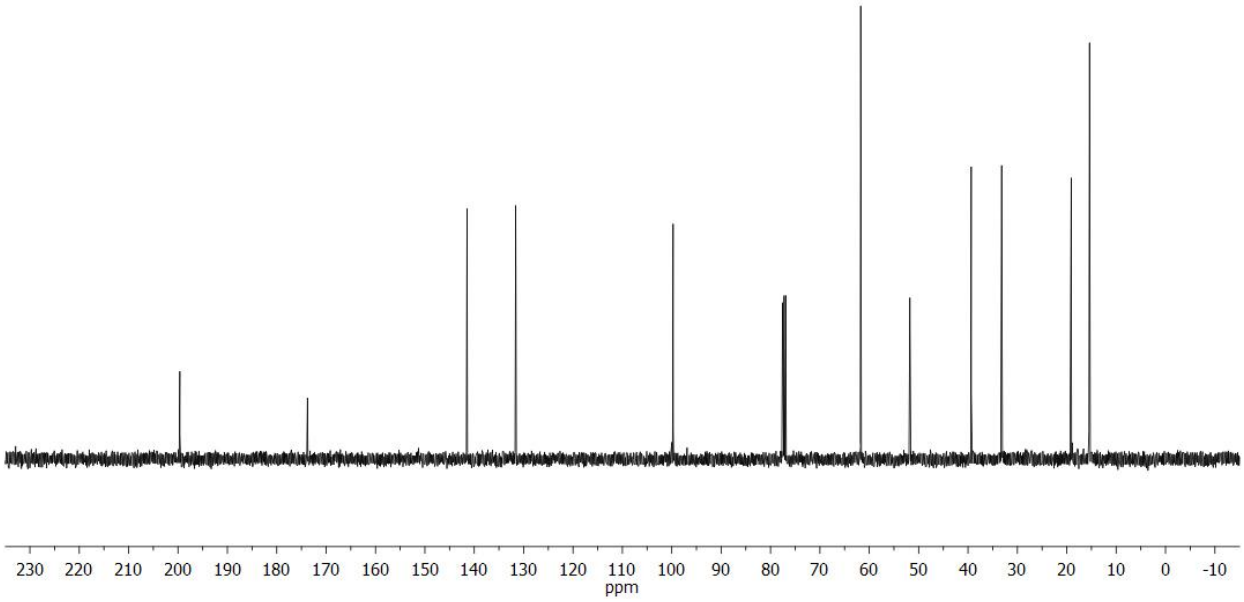

Figure S18 The 100MHz ^{13}C NMR ($CDCl_3$) spectrum of Methyl (*E*)-8,8-diethoxy-5-oxooct-6-enoate (**14b**)

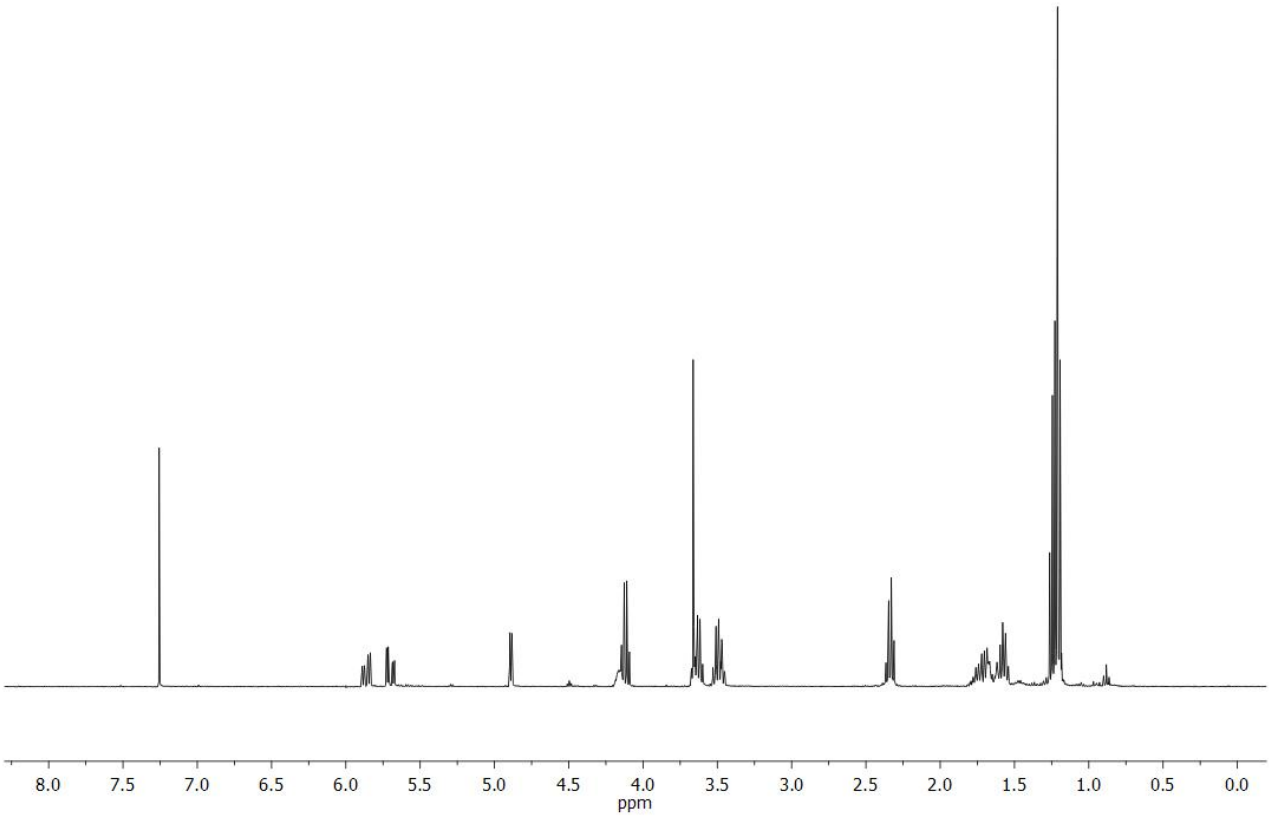

Figure S19 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of Methyl **(***E***)**-8,8-diethoxy-5-hydroxyoct-6-enoate (**15b**)

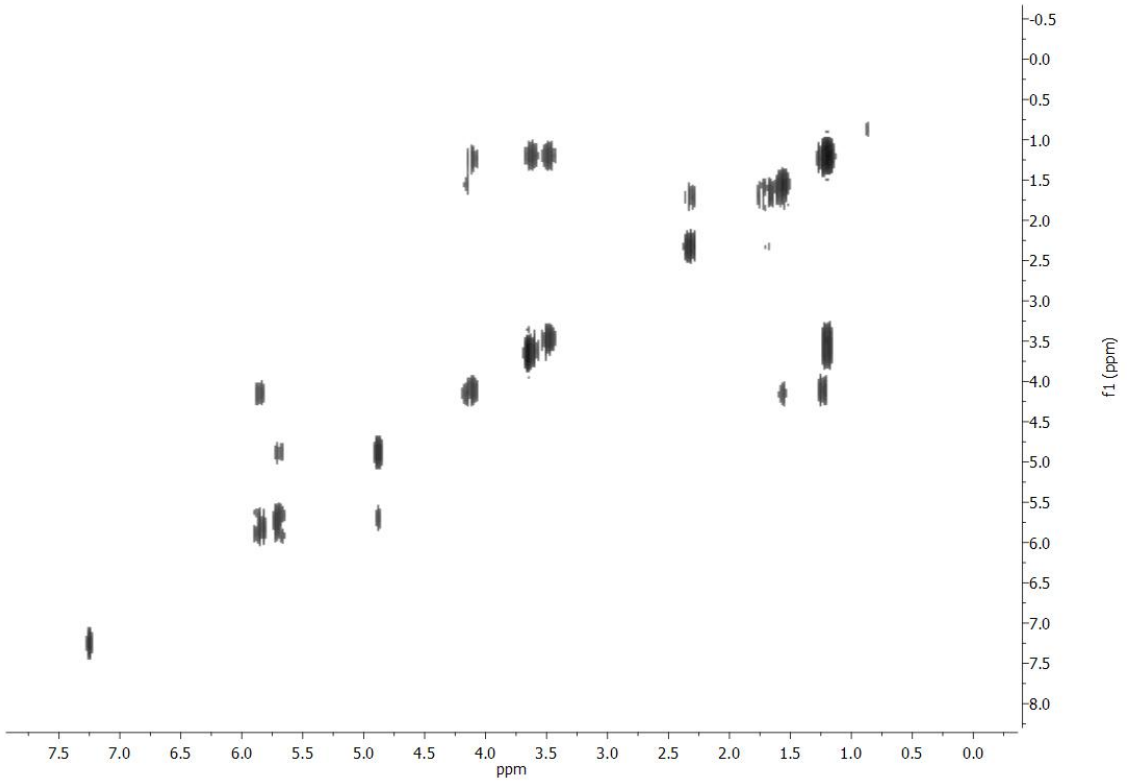

Figure S20 The 400MHz gCOSY ($CDCl_3$) spectrum of Methyl (*E*)-8,8-diethoxy-5-hydroxyoct-6-enoate (**15b**)

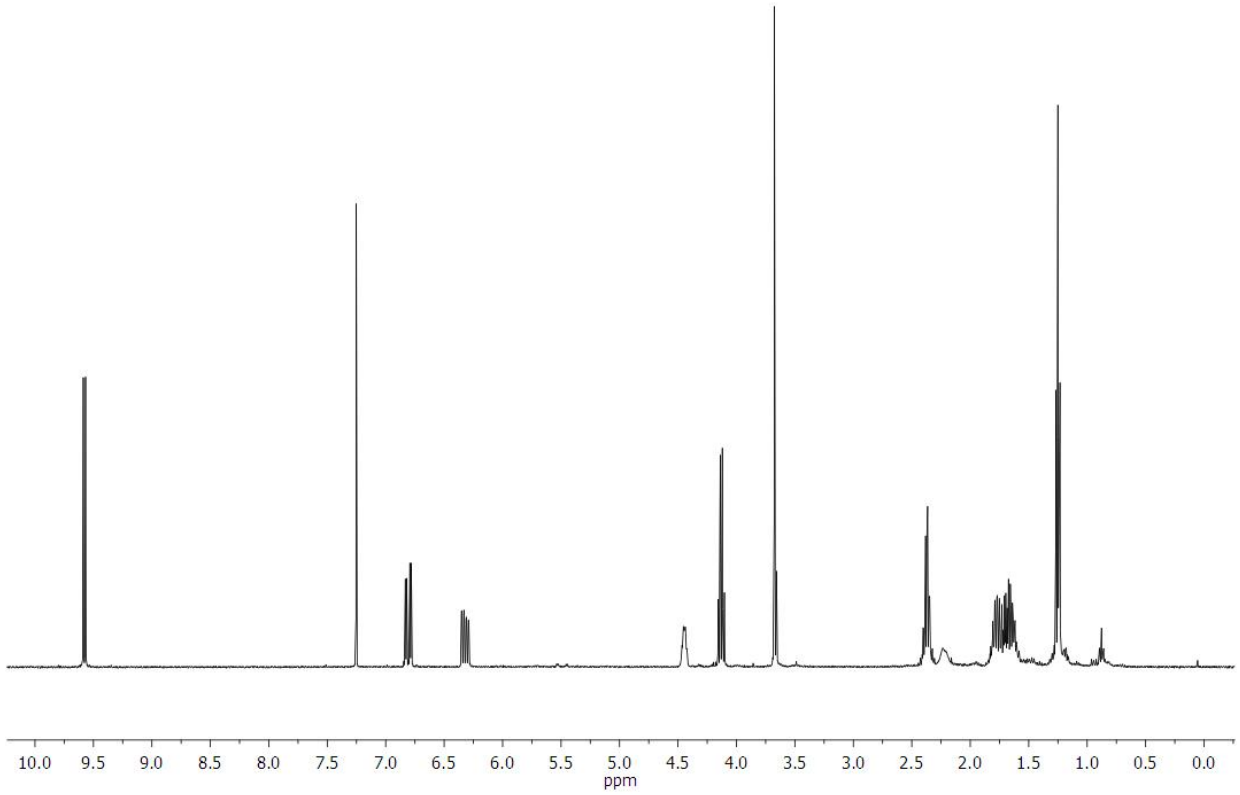

Figure S21 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-methyl-5-hydroxy-8-oxooct-6-enoate (**16**)

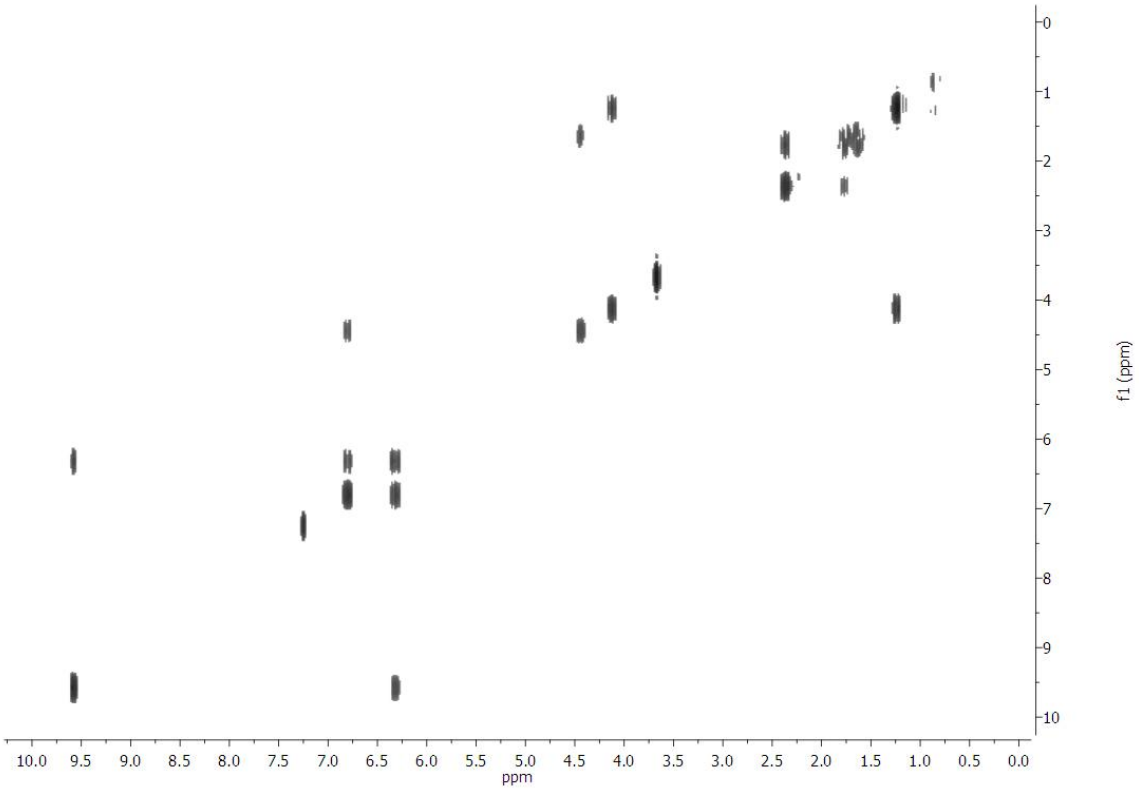

Figure S22 The 400MHz gCOSY NMR ($CDCl_3$) spectrum of (*E*)-methyl-5-hydroxy-8-oxooct-6-enoate (**16**)

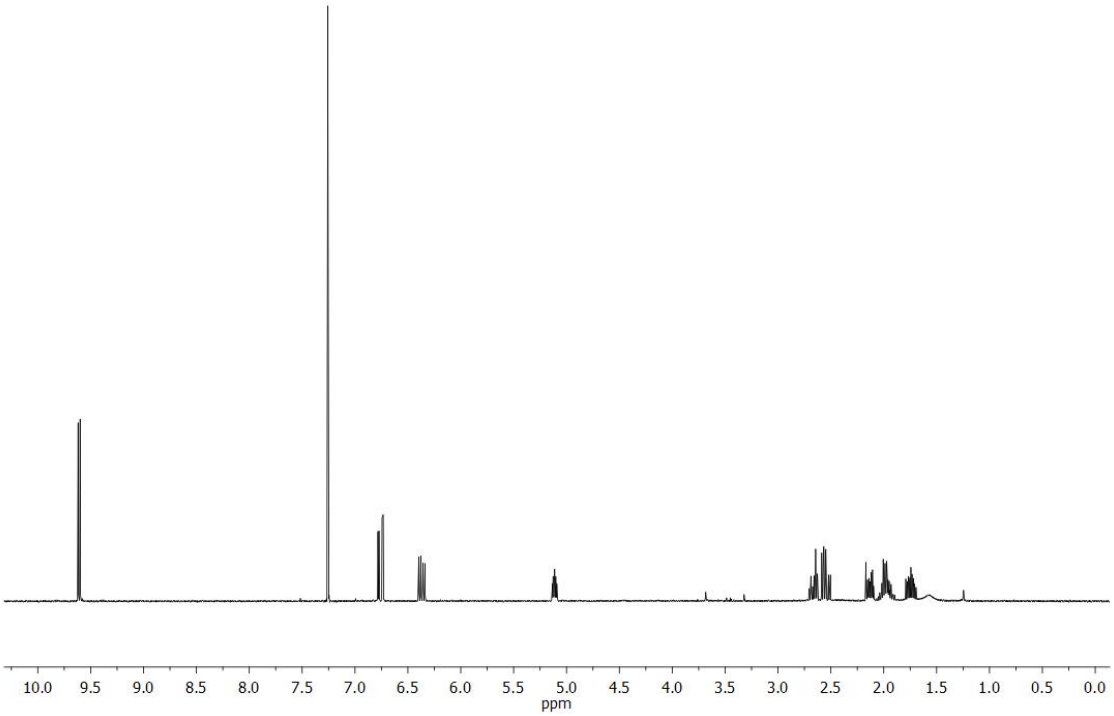

Figure S23 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-3-(6-oxotetrahydro-2H-pyran-2-yl)acrylaldehyde (**17**)

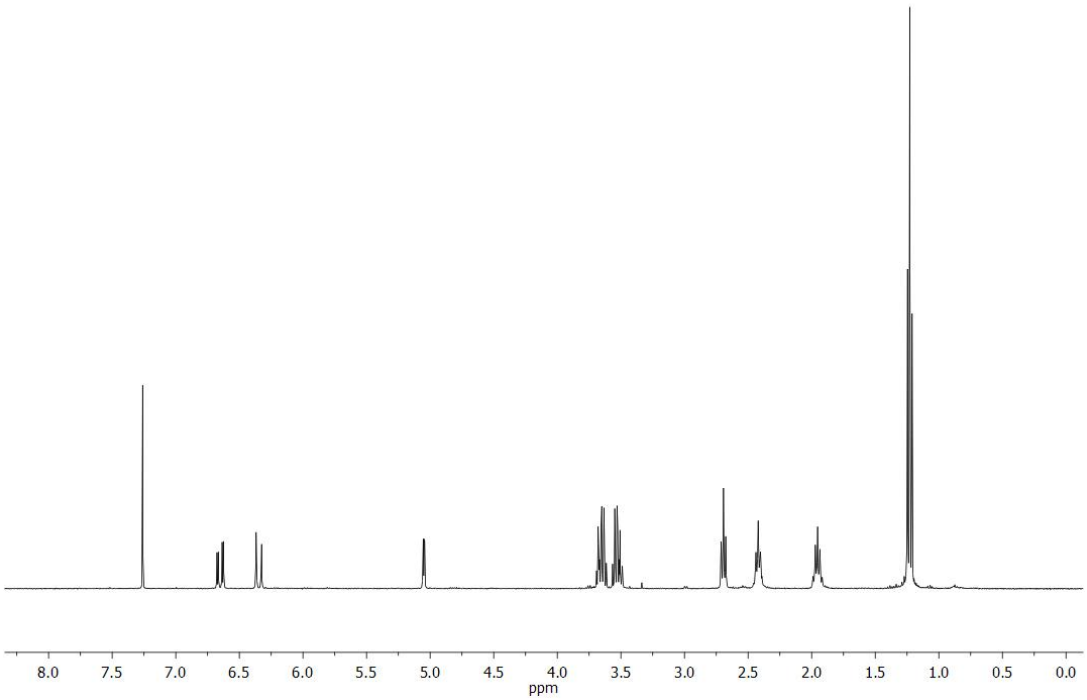

Figure S24 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-8,8-diethoxy-5-oxooct-6-enoic acid (**3b**)

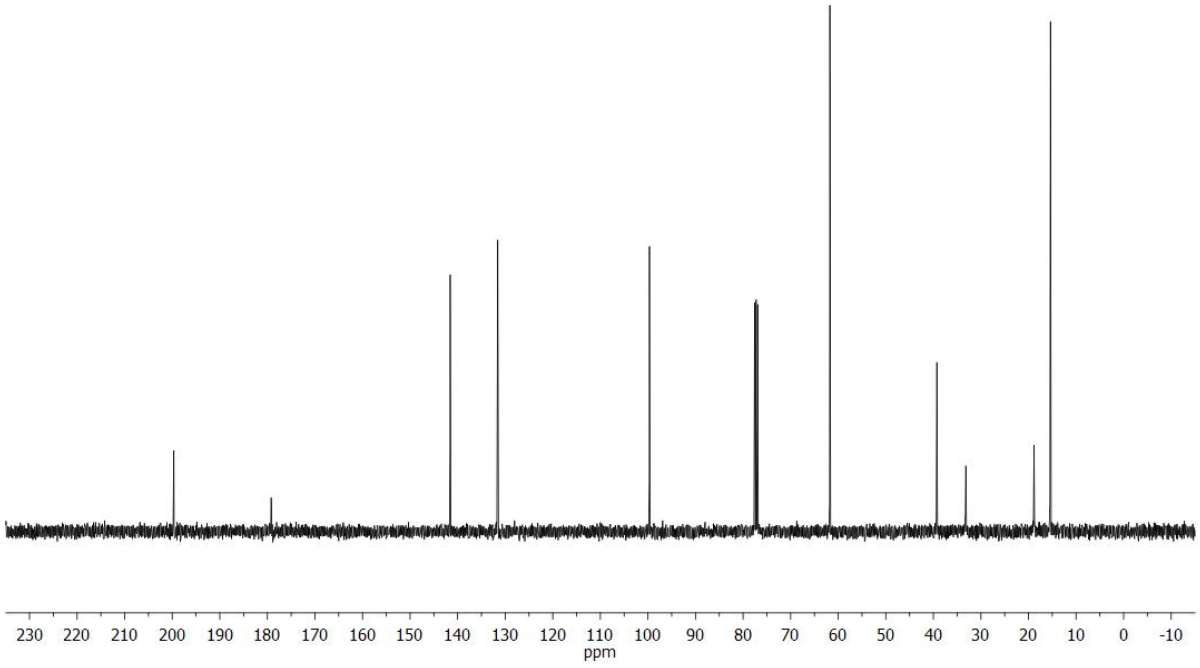

Figure S25 The 100MHz ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-8,8-diethoxy-5-oxooct-6-enoic acid (**3b**)

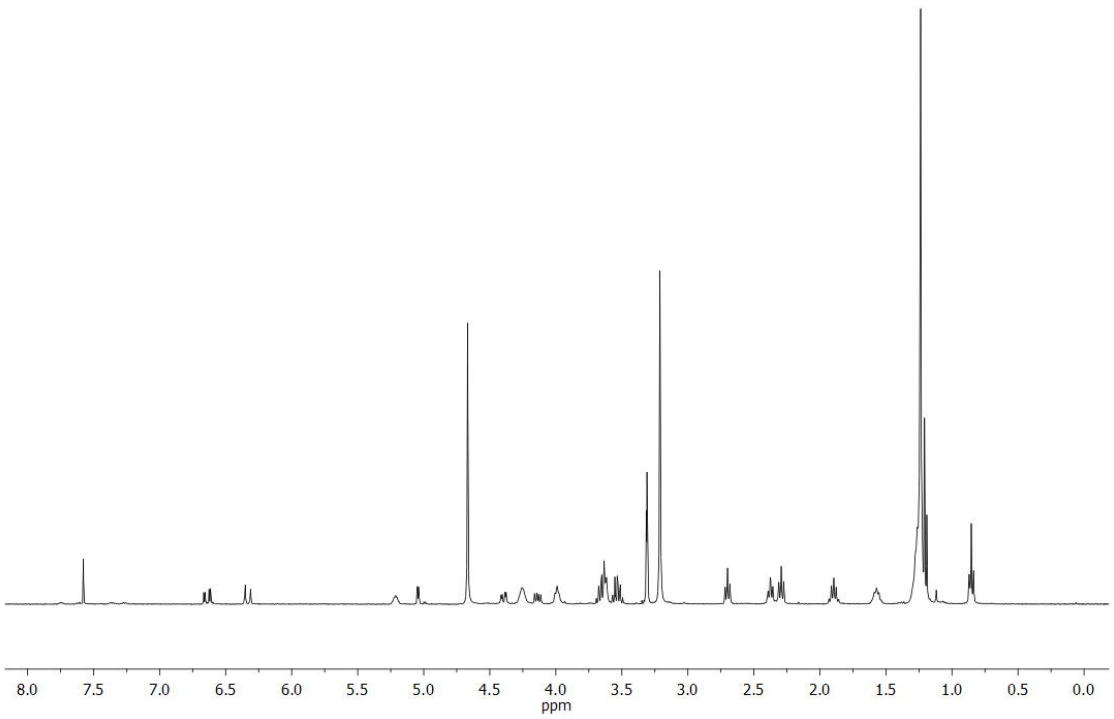

Figure S26 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(8,8-diethoxy-5-oxooct-6-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**18b**)

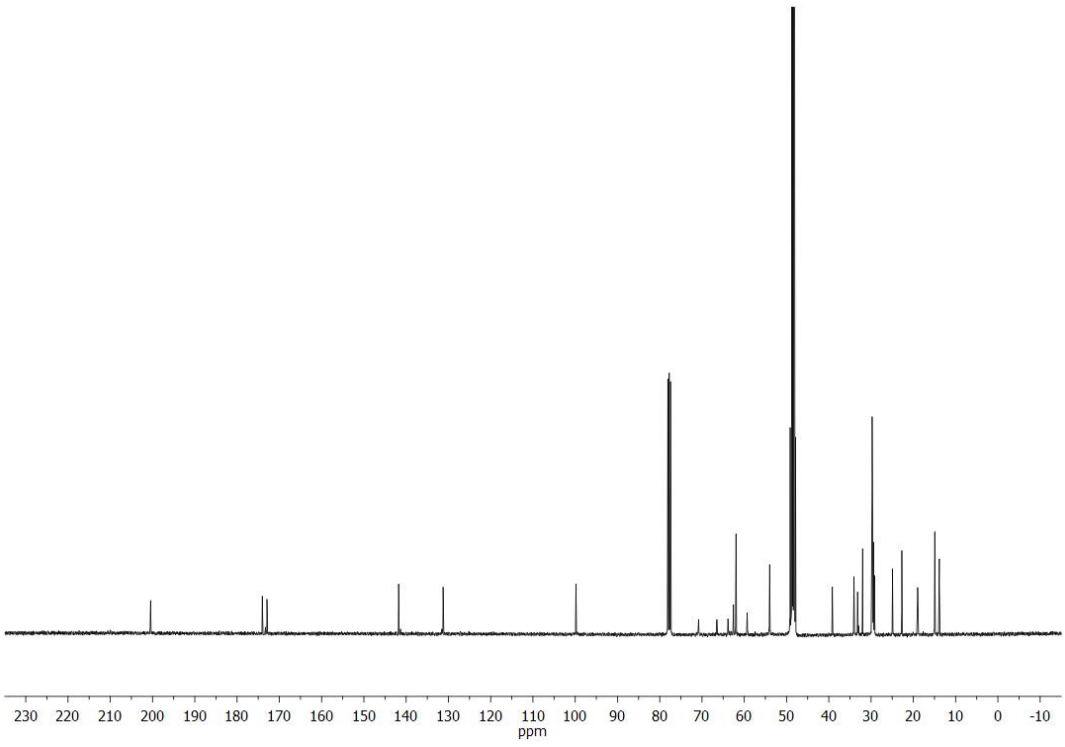

Figure S27 The 100MHz ^{13}C NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(8,8-diethoxy-5-oxooct-6-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**18b**)

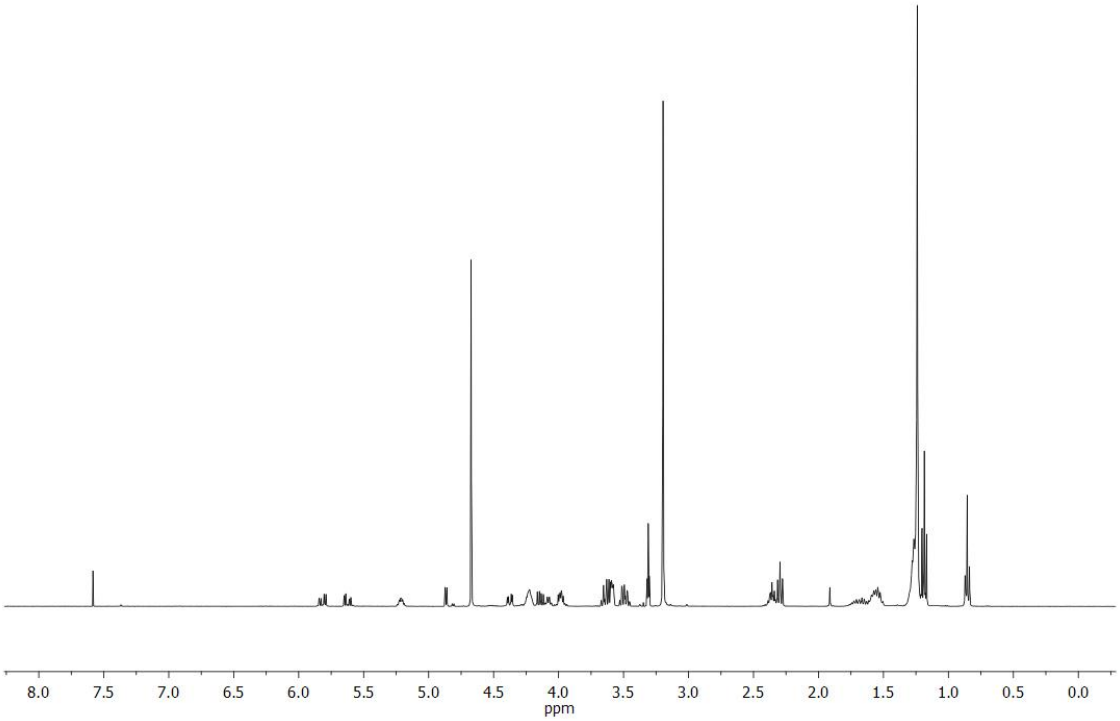

Figure S28 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(5-hydroxy-8,8-diethoxyoct-6-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**2b**)

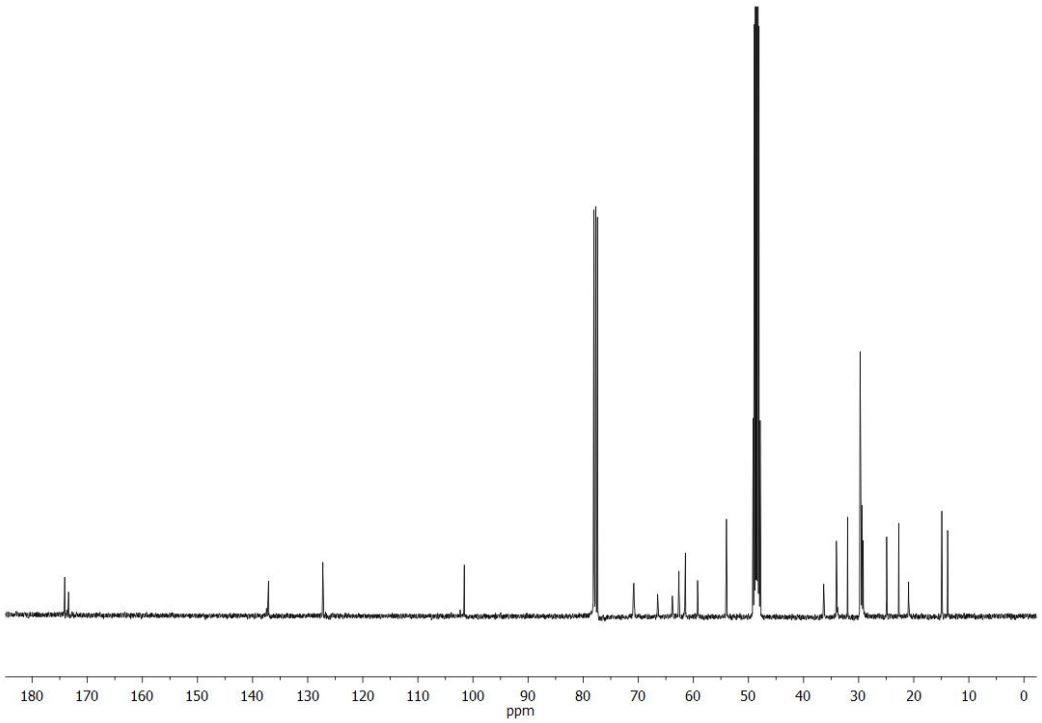

Figure S29 The 100MHz ^{13}C NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(5-hydroxy-8,8-diethoxyoct-6-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**2b**)

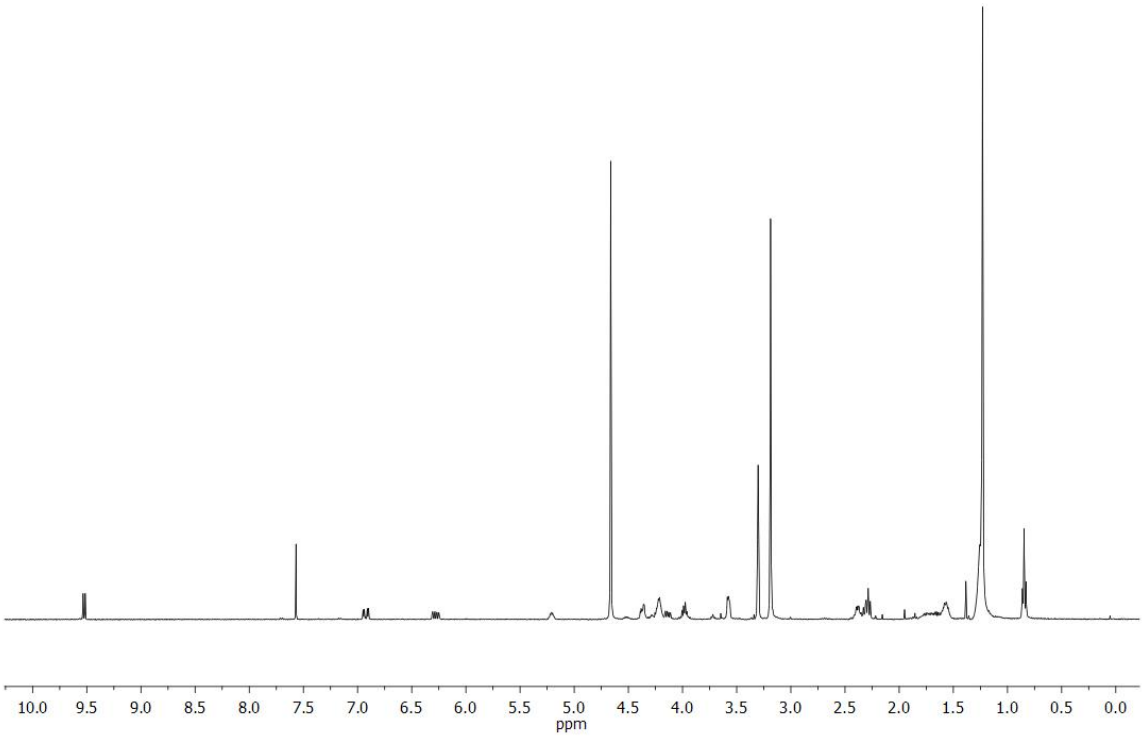

Figure S30 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(5-hydroxy-8-oxooct-6-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**HOOA-PC, 1b**)

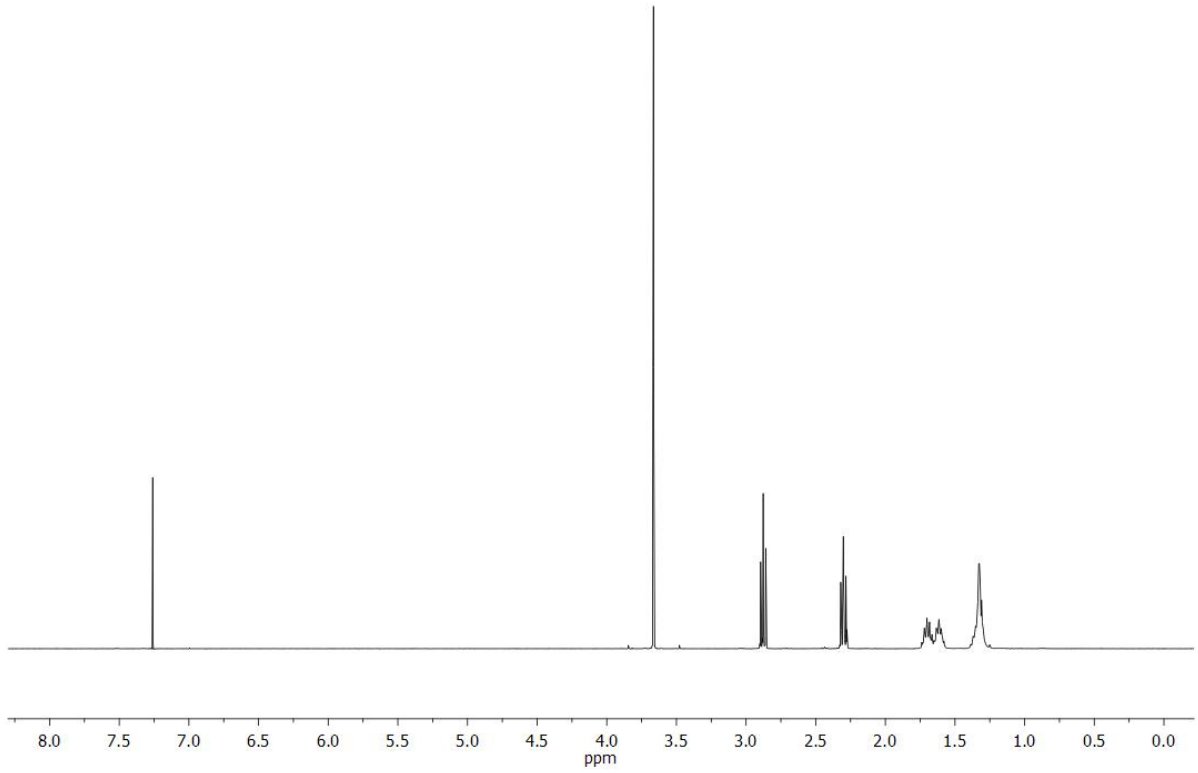

Figure S31 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of Methyl-9-(chlorocarbonyl)octanoate (**7b**)

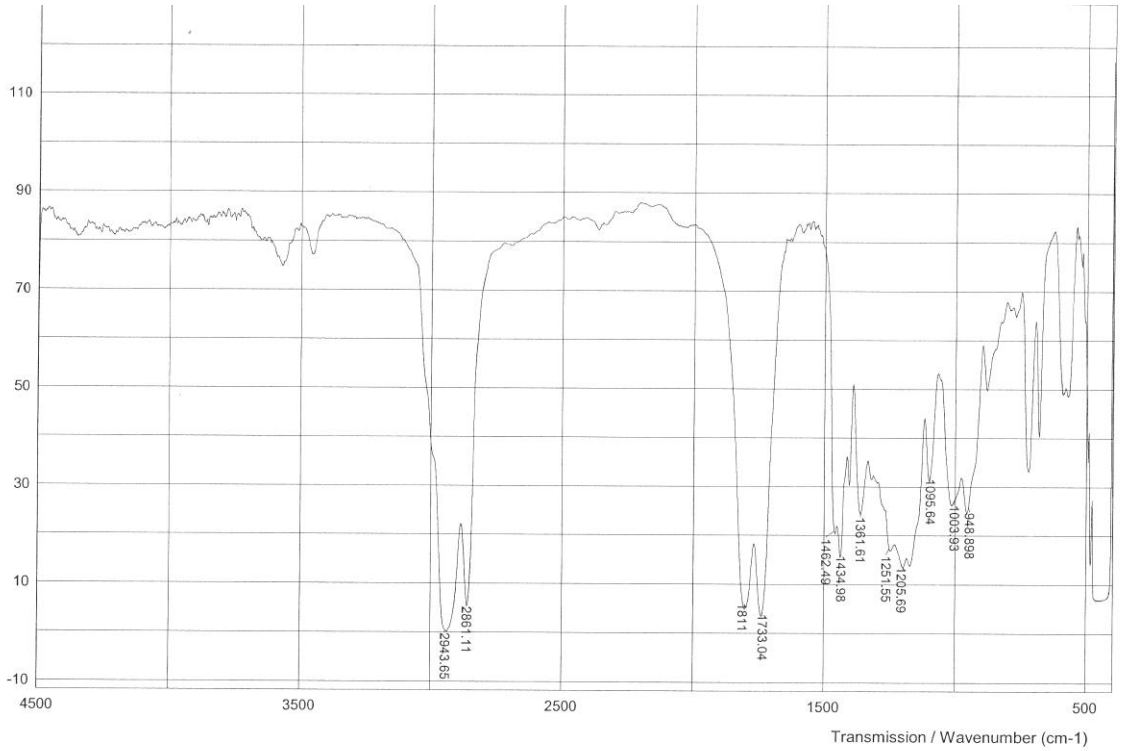

Figure S32 The IR spectrum of Methyl-9-(chlorocarbonyl)octanoate (**7b**)

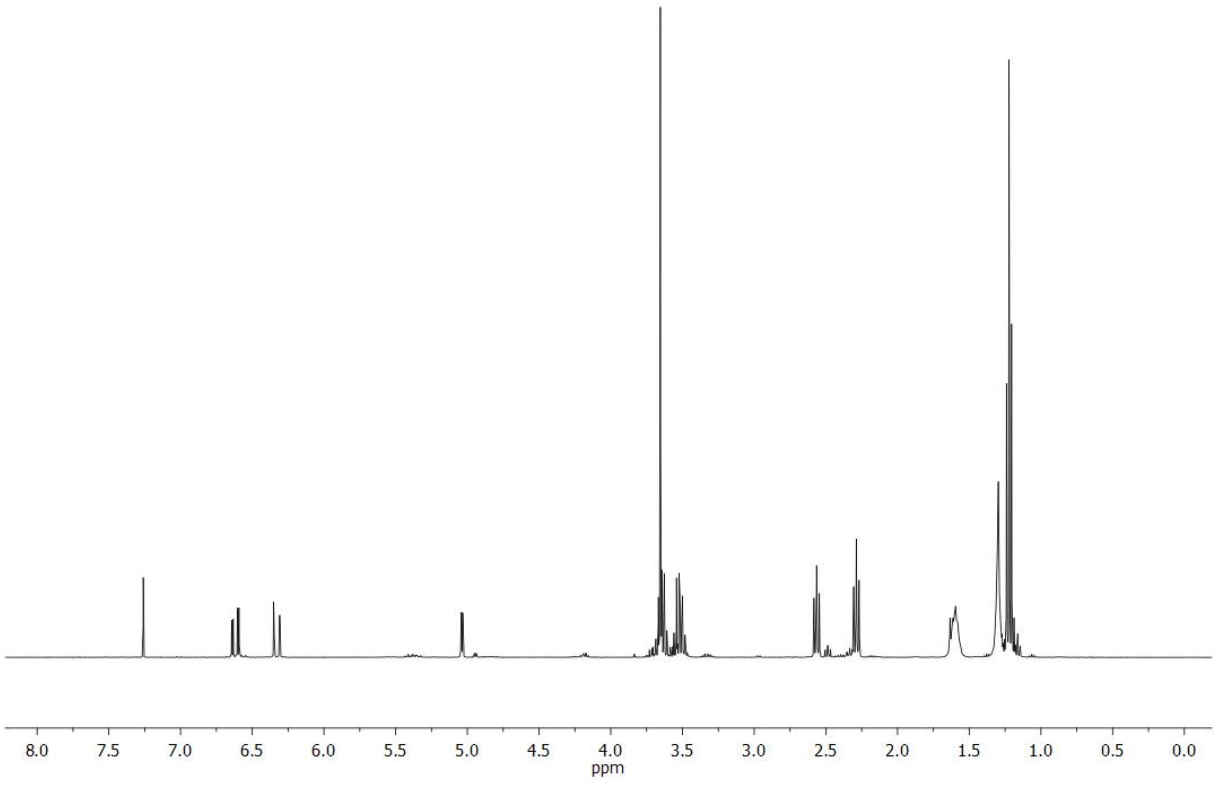

Figure S33 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of Methyl (*E*)-12,12-diethoxy-9-oxodec-10-enoate (**14c**)

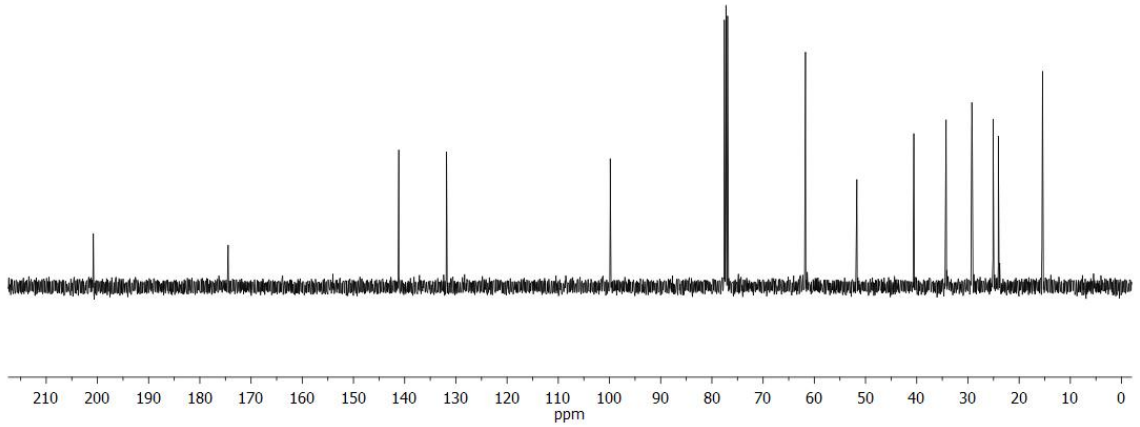

Figure S34 The 100MHz ^{13}C NMR ($CDCl_3$) spectrum of Methyl (*E*)-12,12-diethoxy-9-oxodec-10-enoate (**14c**)

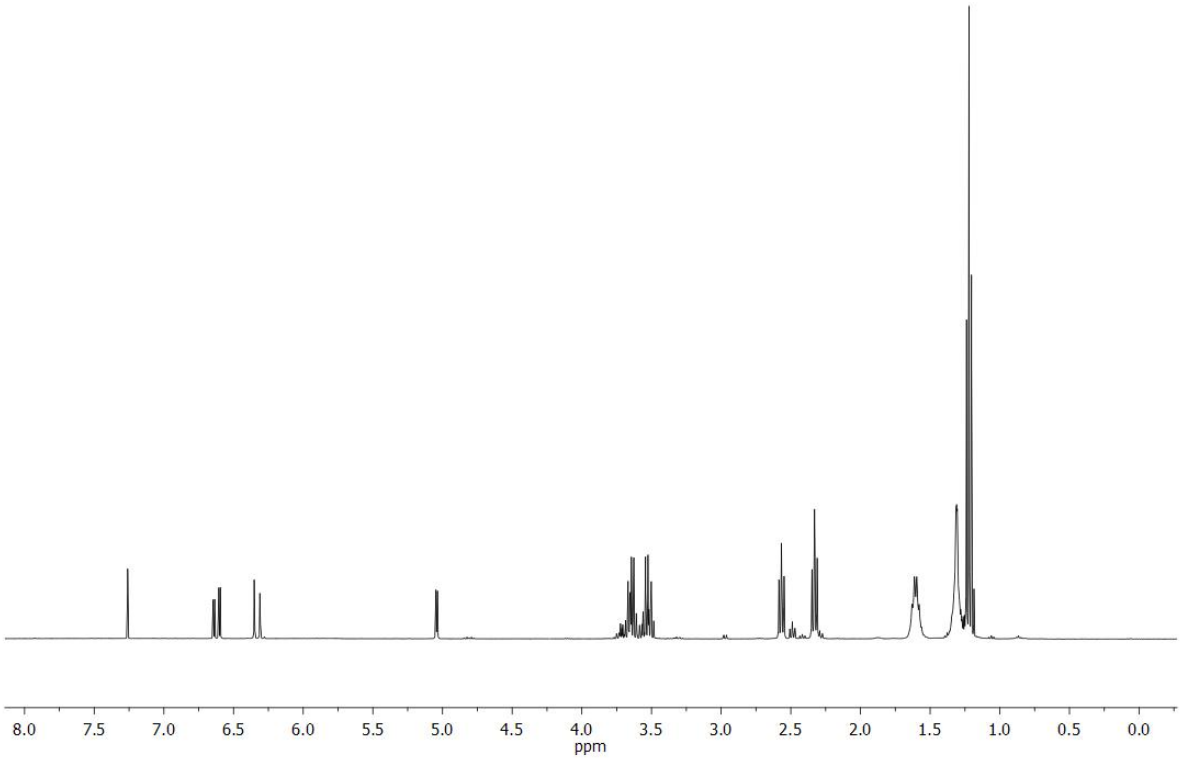

Figure S35 The 400MHz ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-12,12-diethoxy-9-oxodec-10-enoic acid (**3c**)

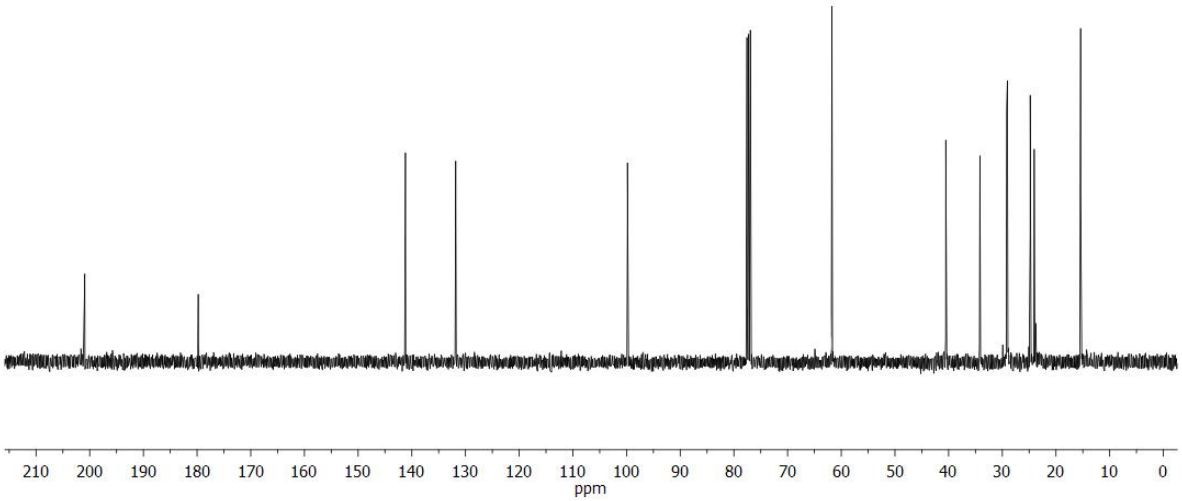

Figure S36 The 100MHz ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-12,12-diethoxy-9-oxodec-10-enoic acid (**3c**)

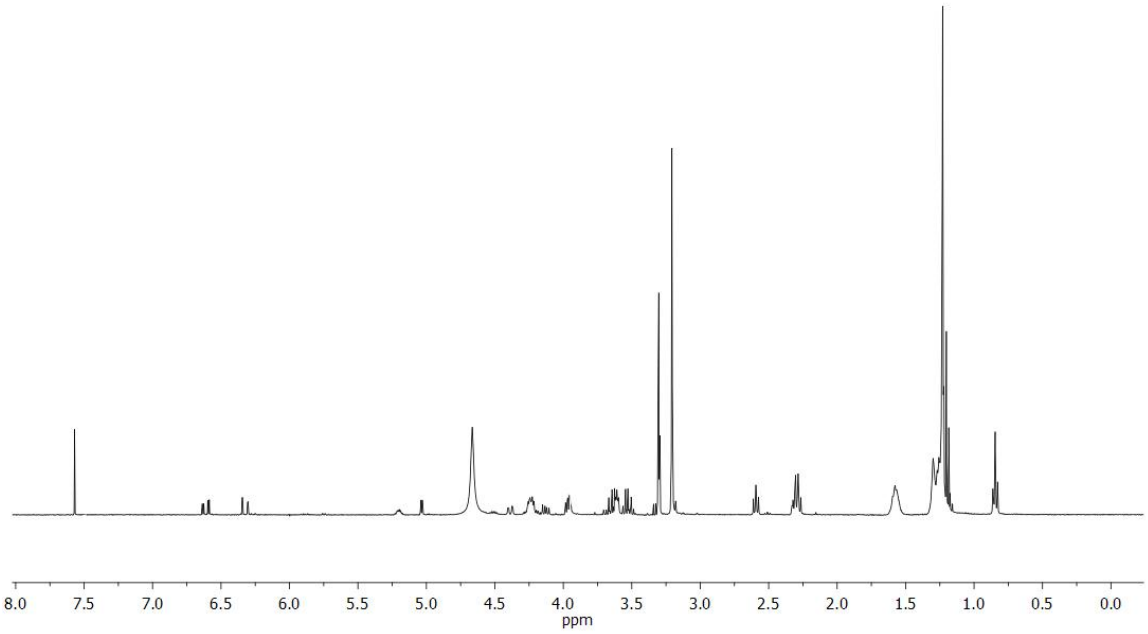

Figure S37 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(12,12-diethoxy-9-oxodec-10-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**18c)**

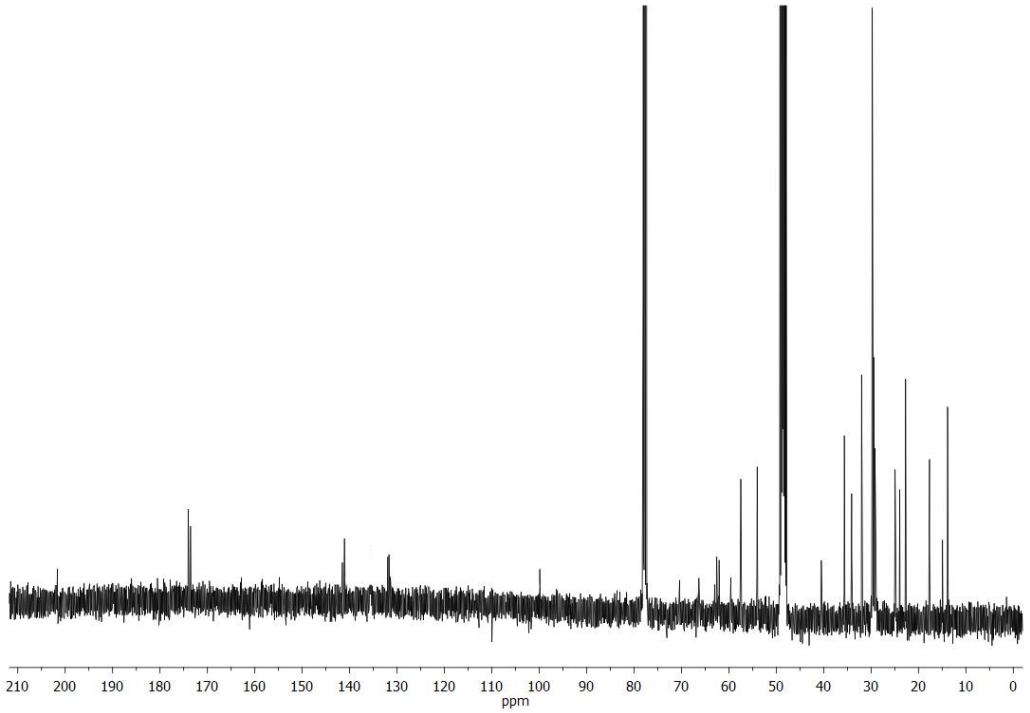

Figure S38 The 100MHz ^{13}C NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(12,12-diethoxy-9-oxodec-10-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**18c**)

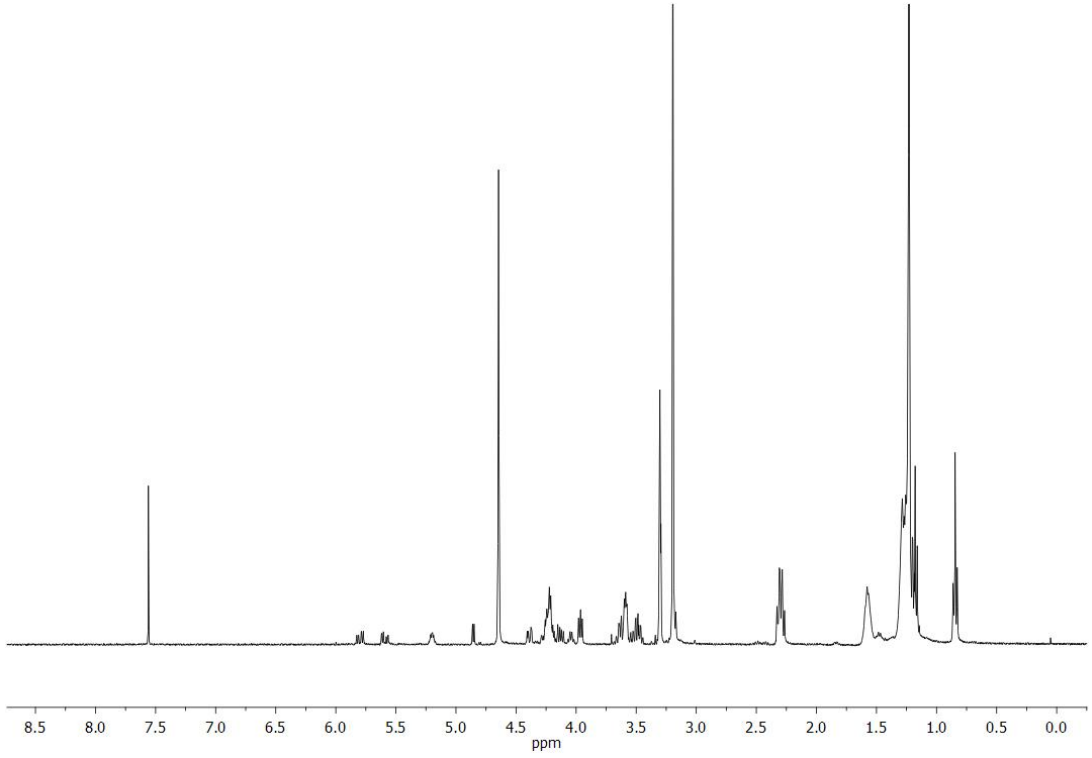

Figure S39 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(9-hydroxy-12,12-diethoxydec-10-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**2c**)

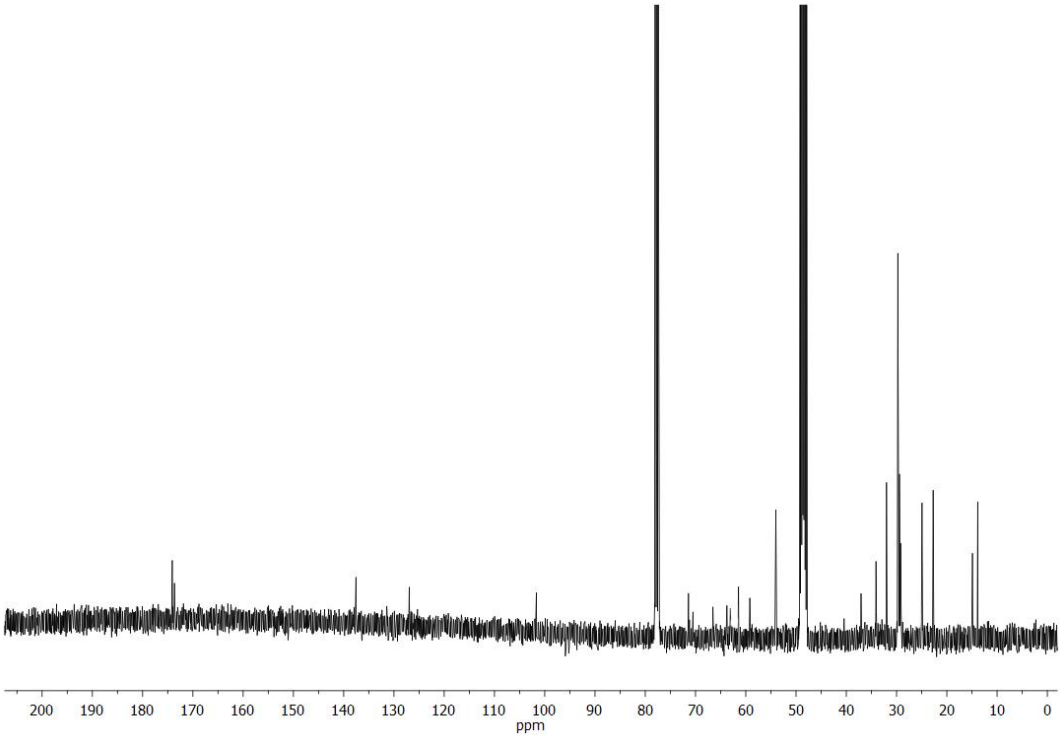

Figure S40 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(9-hydroxy-12,12-diethoxydec-10-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**2c**)

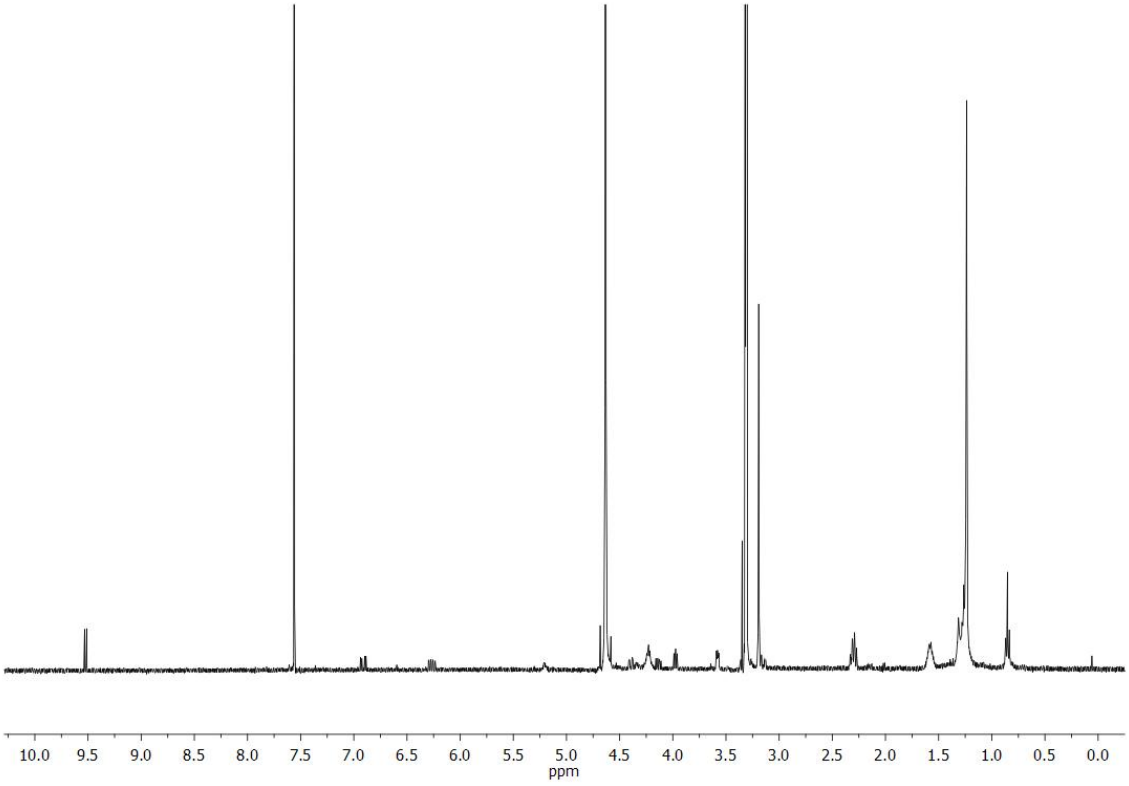

Figure S41 The 400MHz ^{1}H NMR (CD_3OD+$CDCl_3$) spectrum of (*E*)-(9-hydroxy-12-oxodec-10-enoyl)-1-palmitoyl-*sn*-glycero-3-phosphatidylcholine (**HODA-PC, 1c**)