

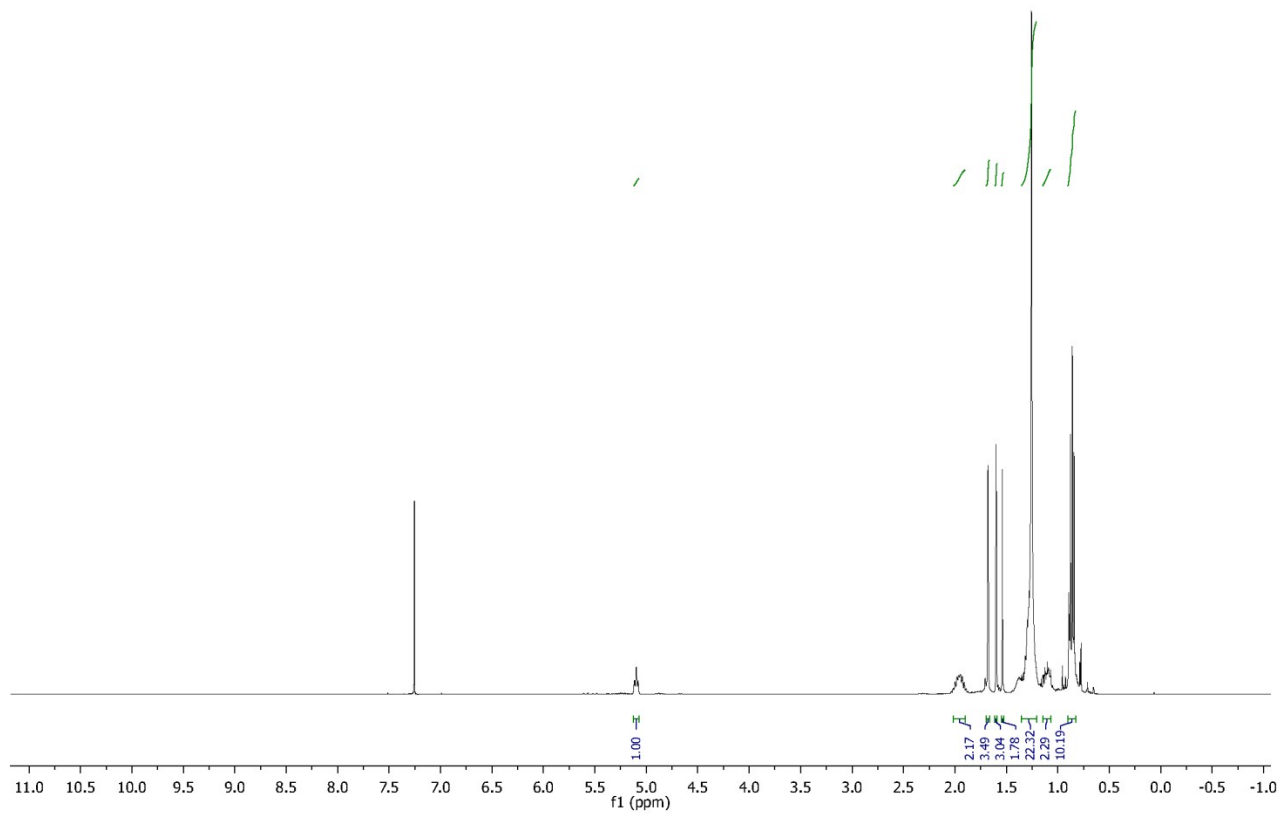
Total synthesis and mass spectrometric analysis of a *Mycobacterium tuberculosis* phosphatidylglycerol featuring a two-step synthesis of (*R*)-tuberculostearic acid

Satvika Burugupalli, Mark B. Richardson, Spencer J. Williams*

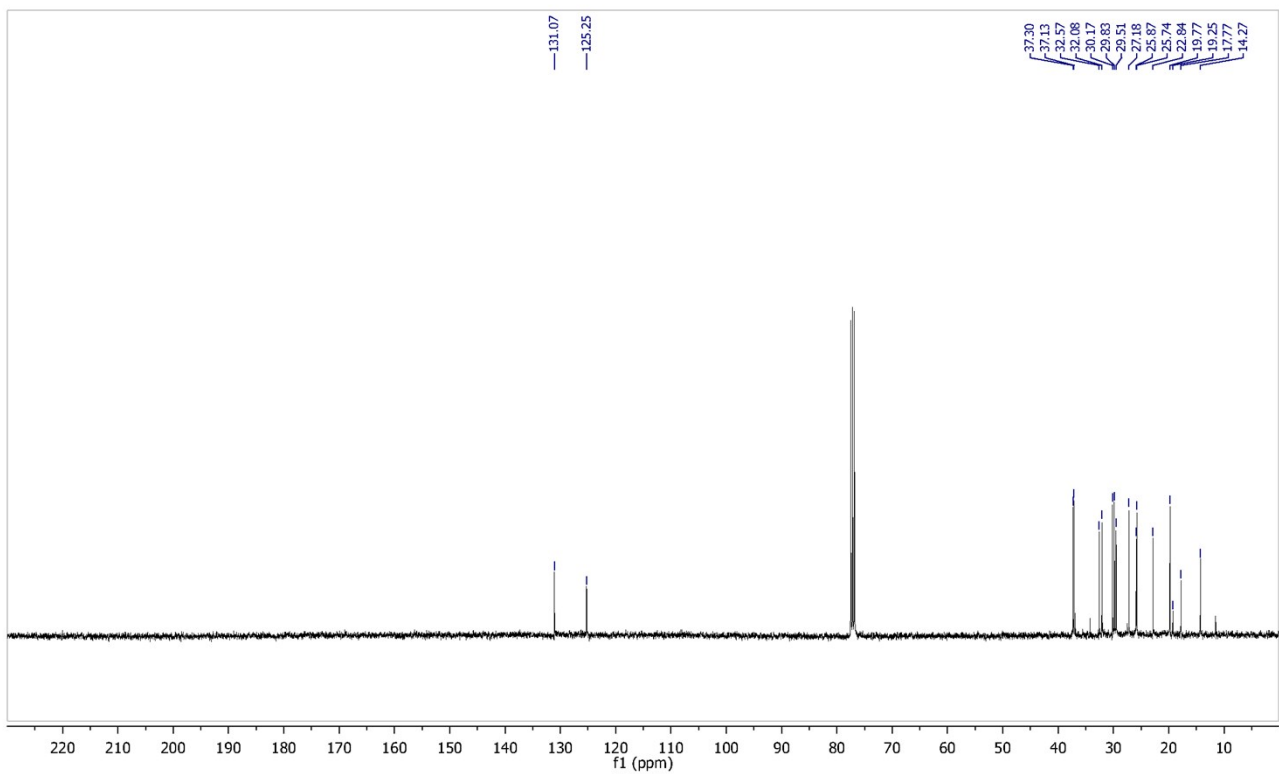
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NMR spectra
(*R*)-2,6-Dimethyltetradecene (4)
¹H NMR

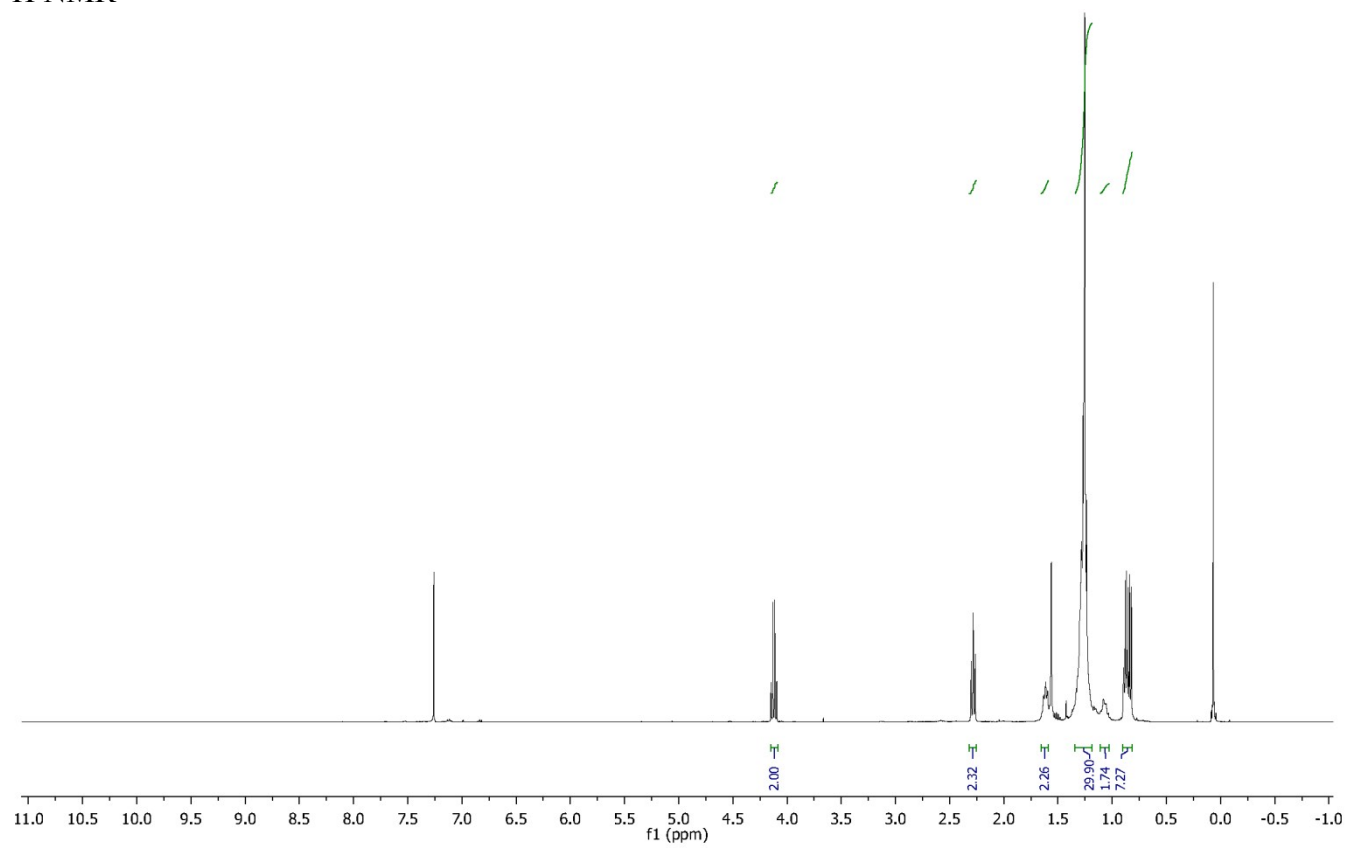


¹³C NMR

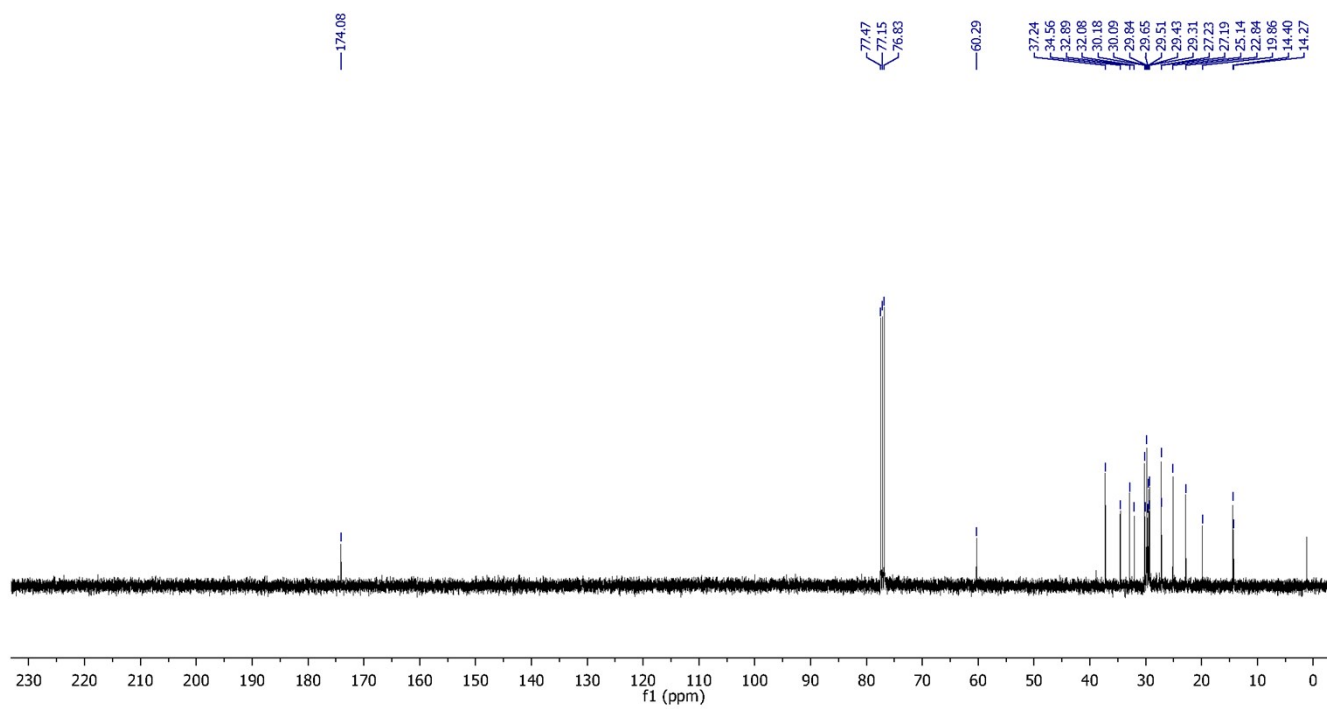


Ethyl (*R*)-10-methyloctadecanoate

^1H NMR

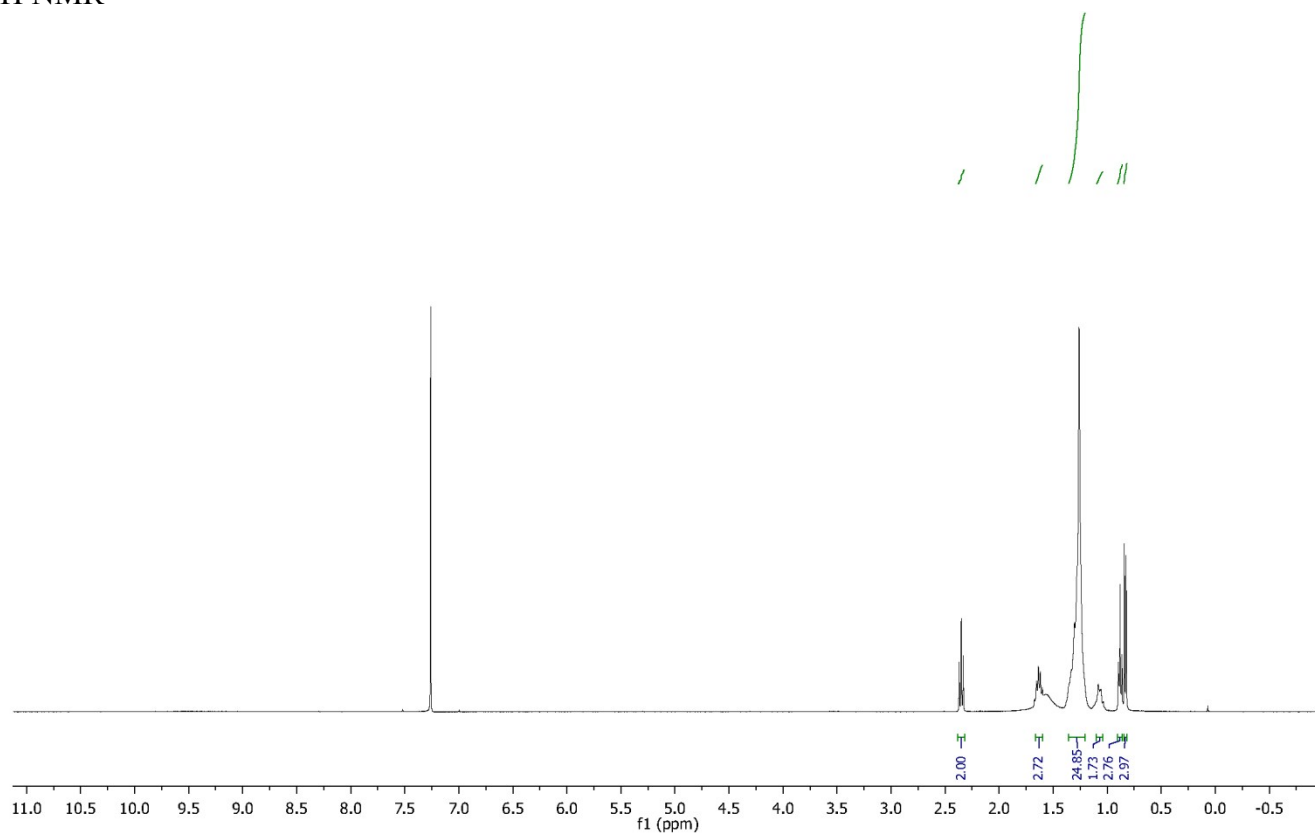


^{13}C NMR

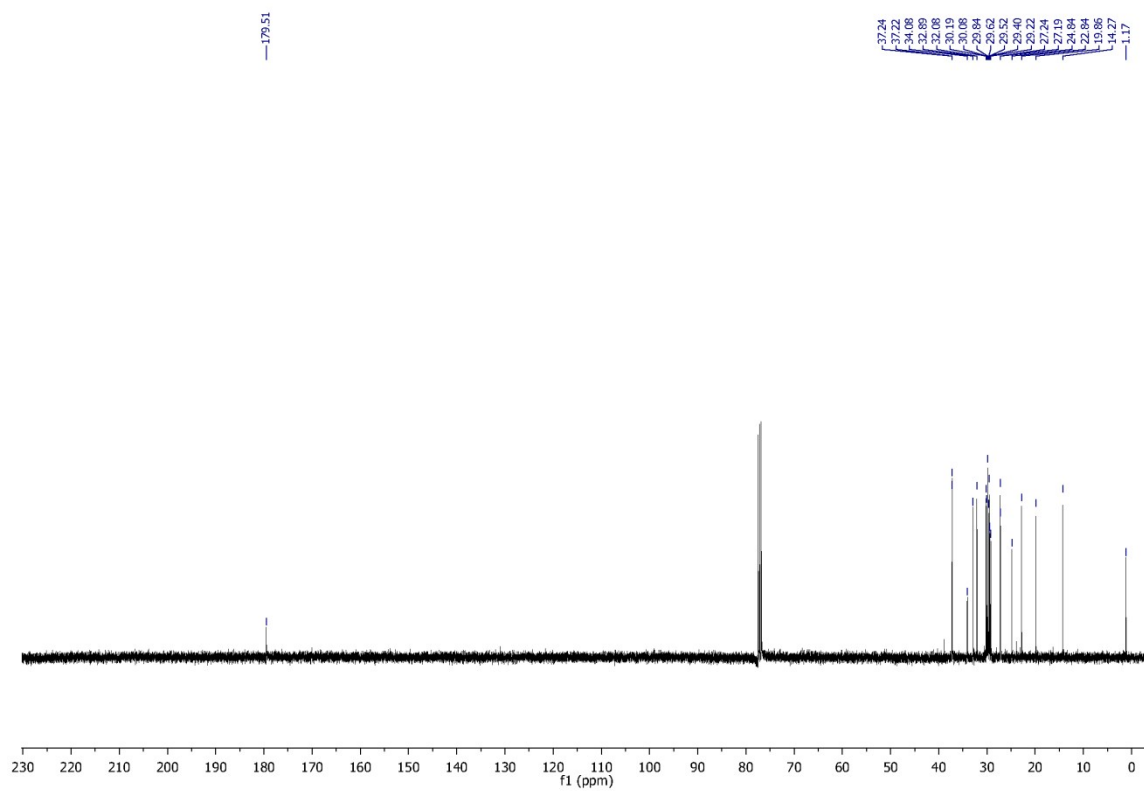


(R)-10-Methyloctadecanoic acid (2)

¹H NMR

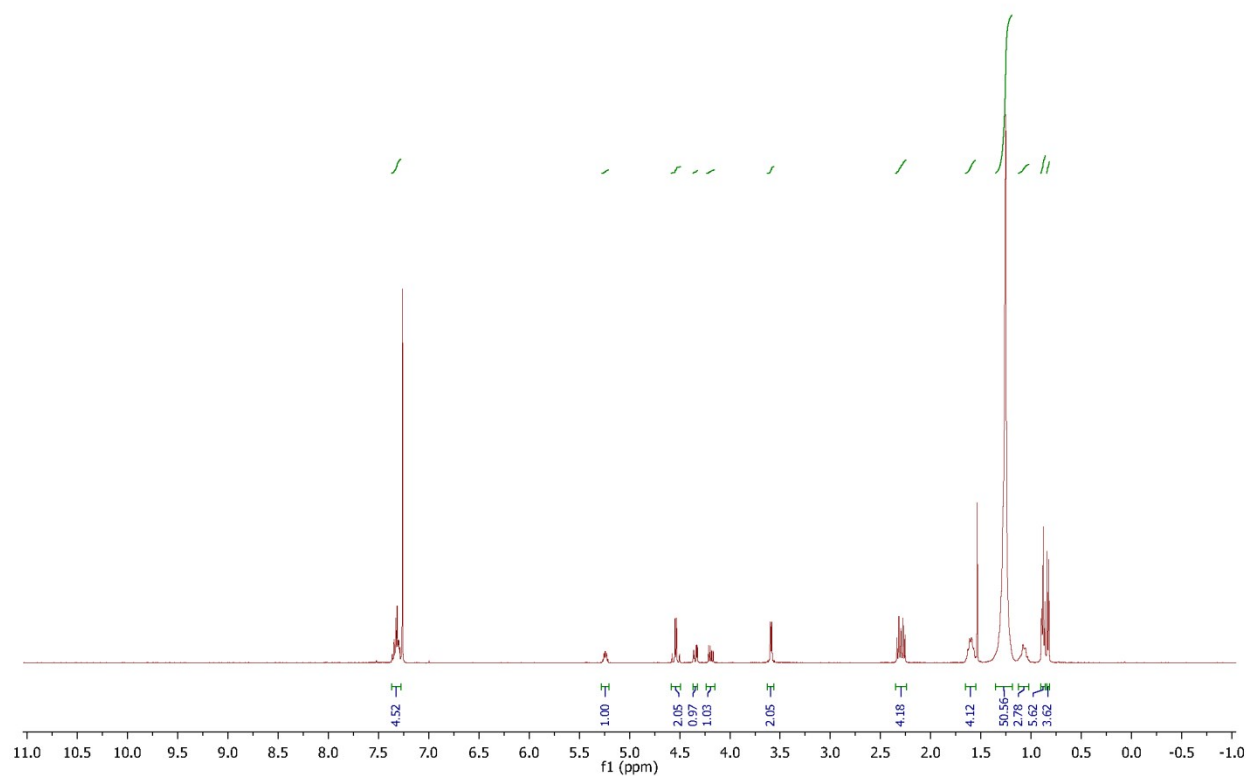


¹³C NMR

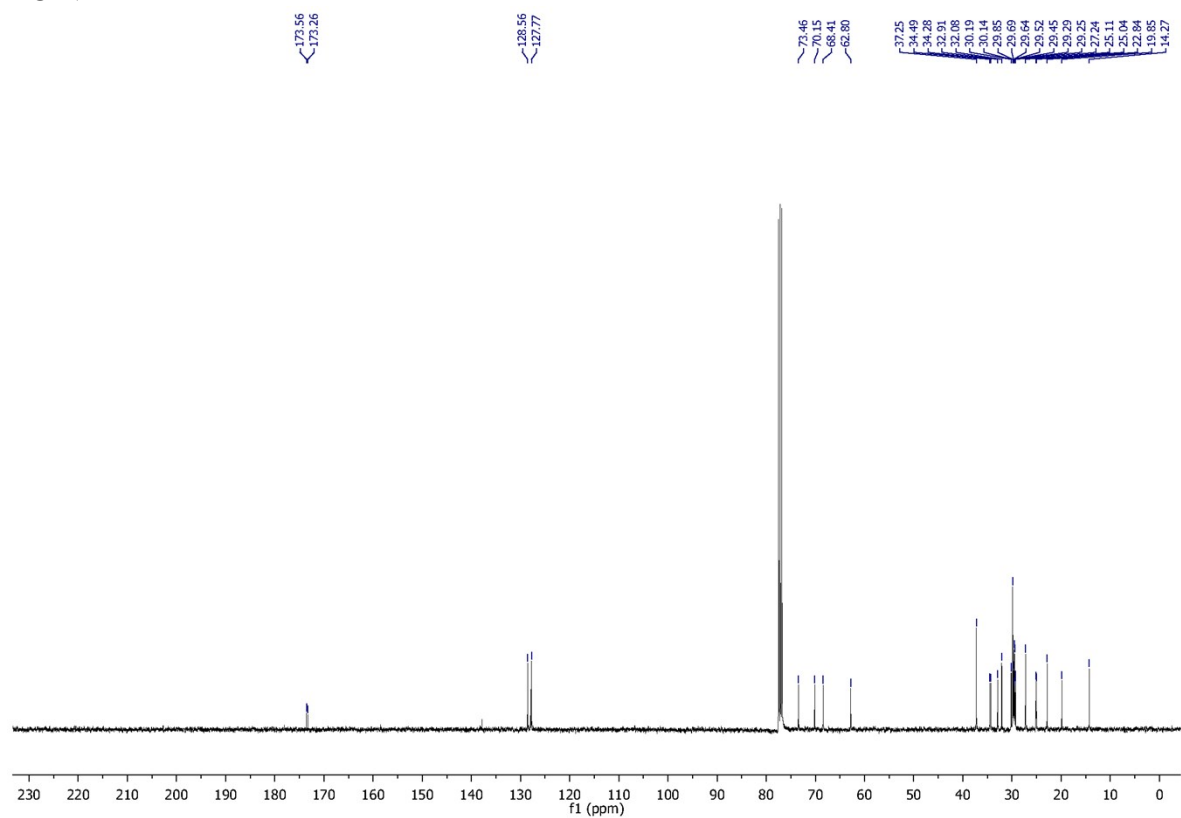


3-*O*-Benzyl-1-*O*-((*R*)-10-methyloctadecanoyl)-2-*O*-palmitoyl-sn-glycerol (6c)

¹H NMR

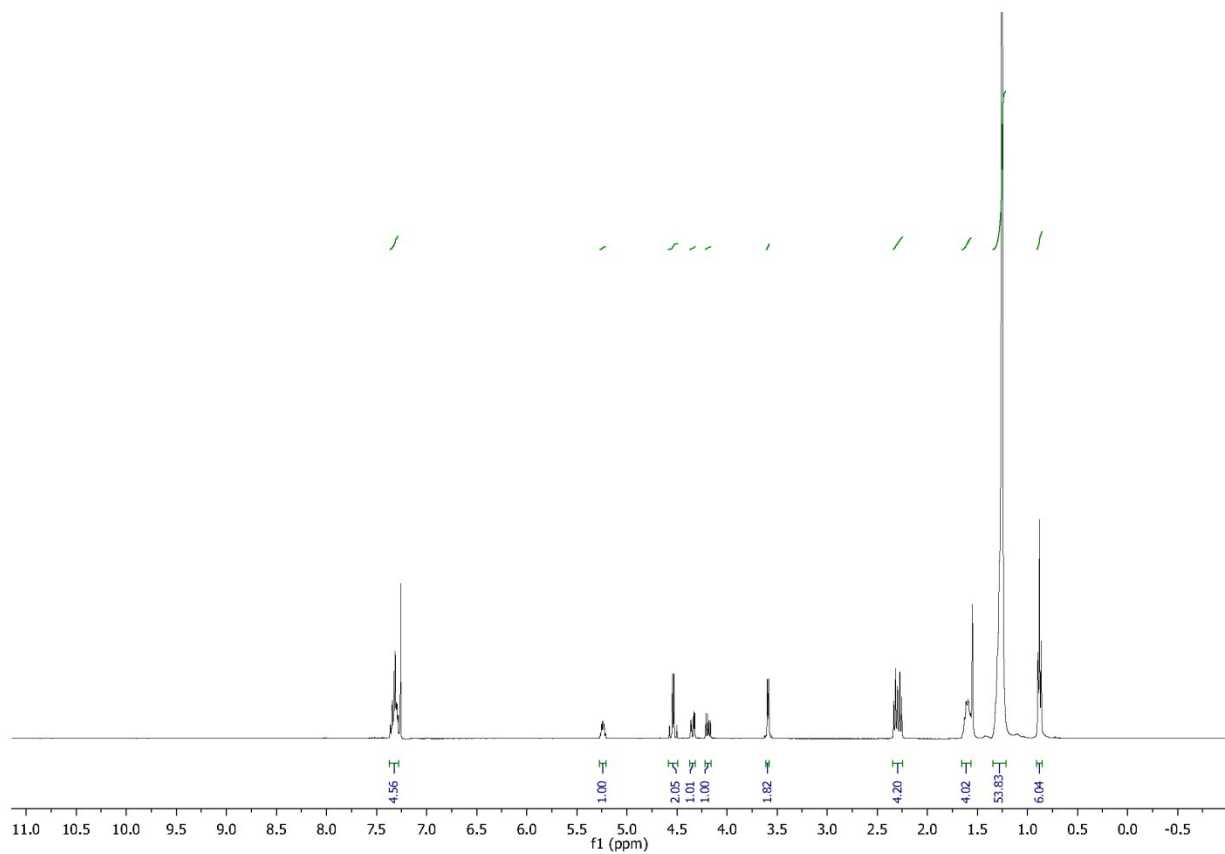


¹³C NMR

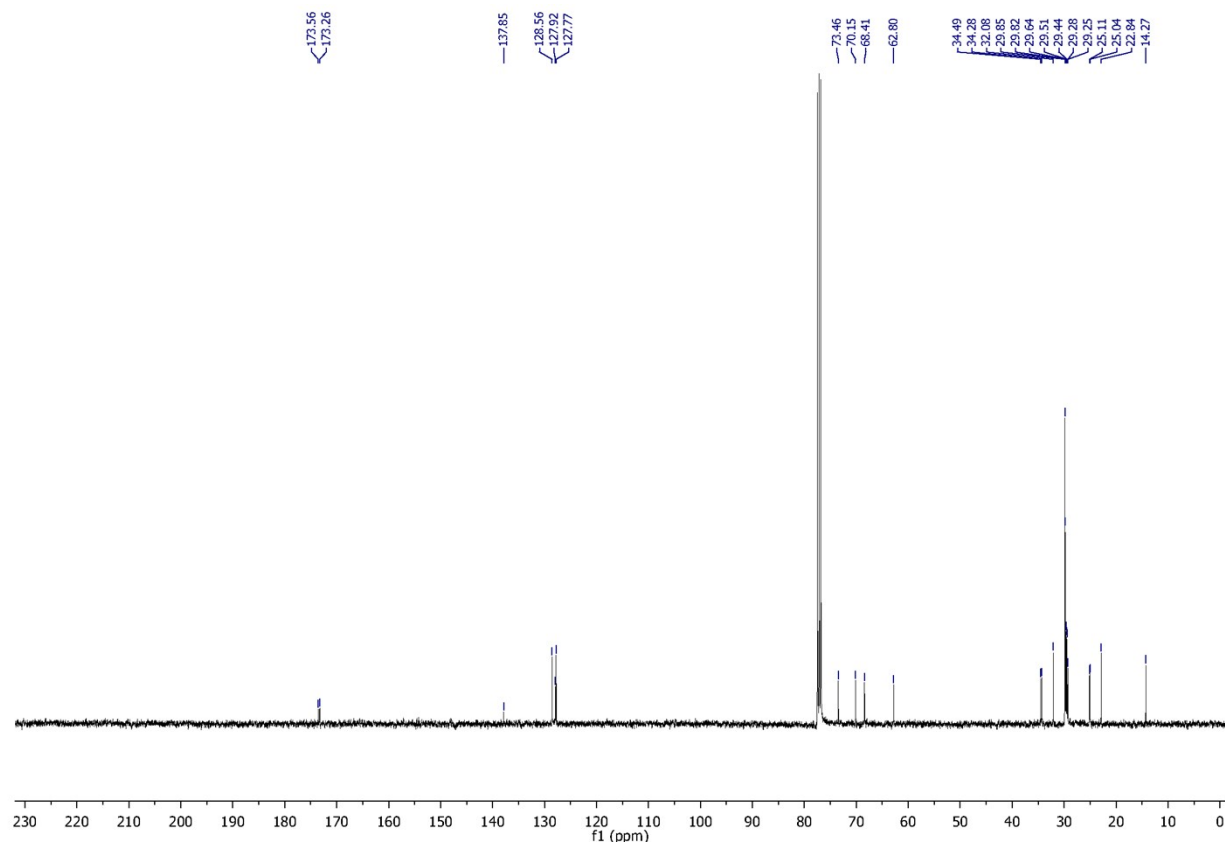


3-*O*-Benzyl-1-*O*-palmitoyl-2-*O*-stearoyl-sn-glycerol (6a)

^1H NMR

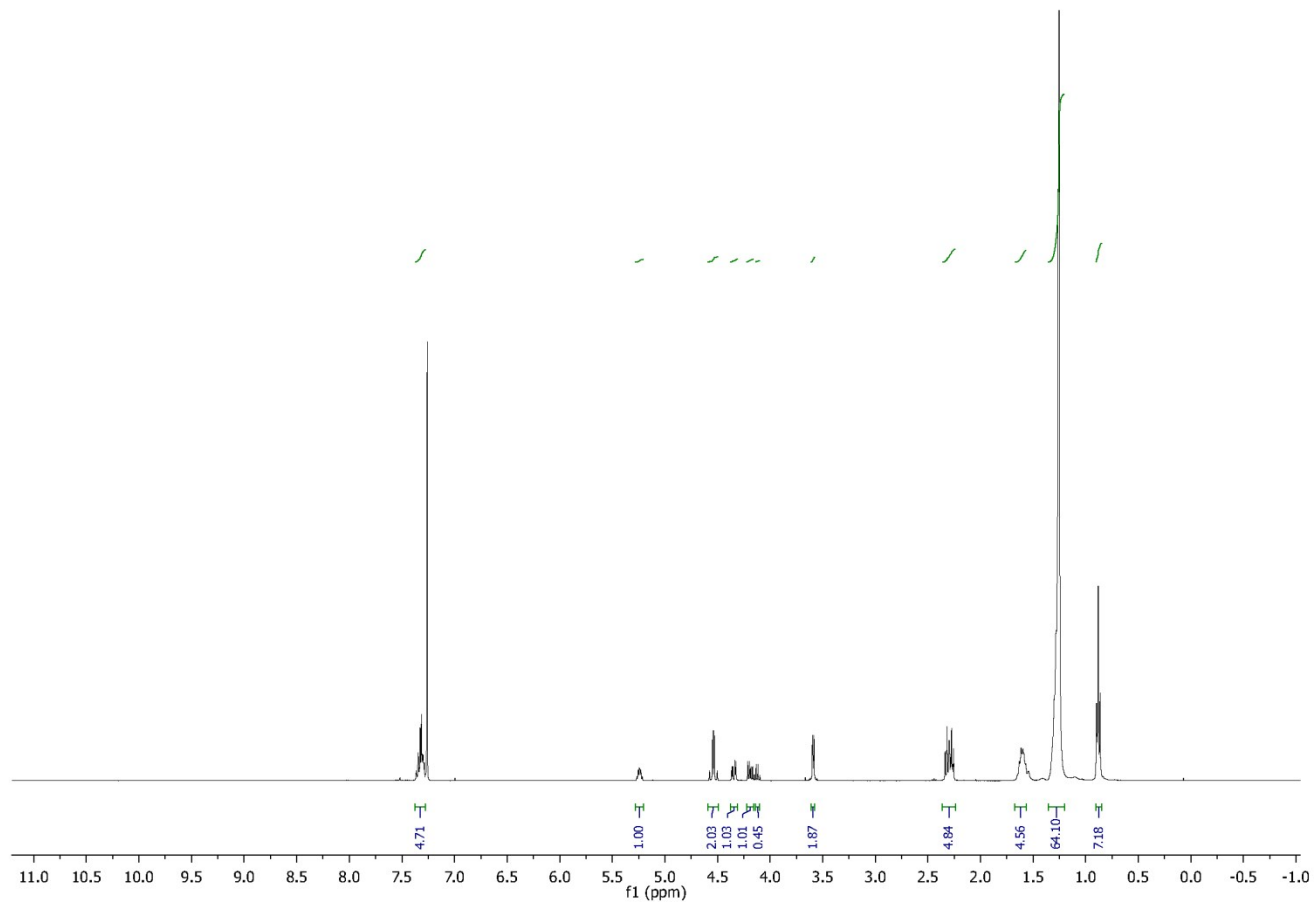


^{13}C NMR

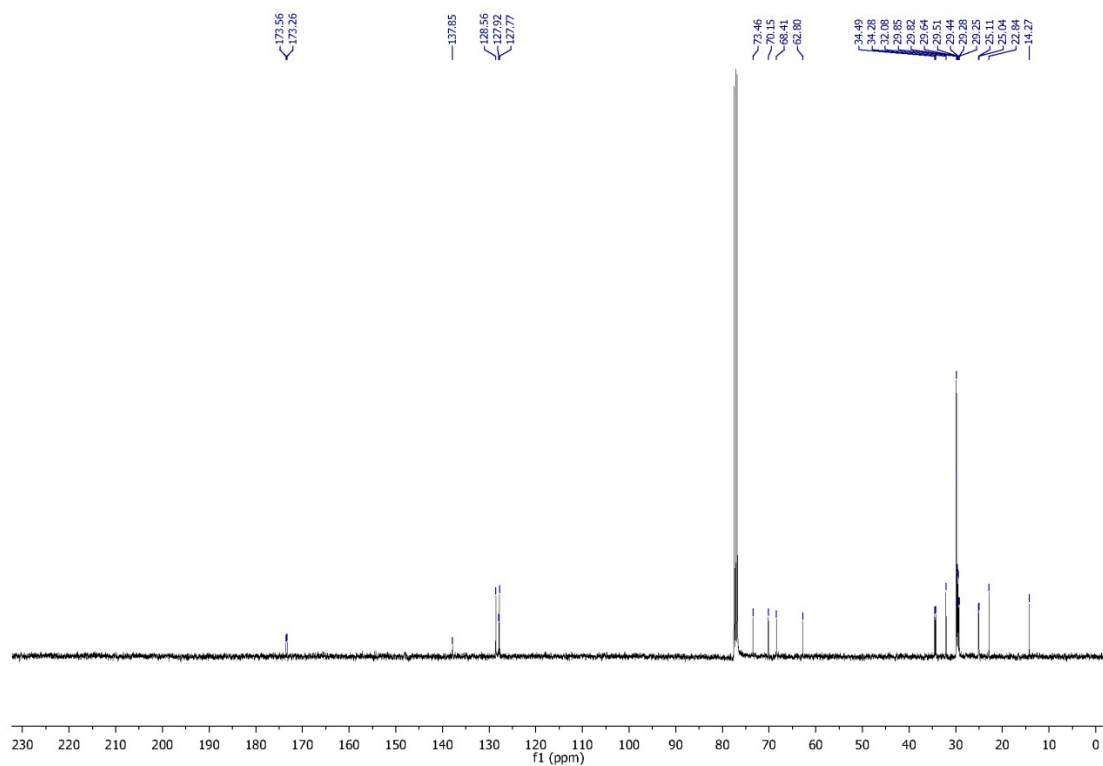


3-*O*-Benzyl-1-*O*-stearoyl-2-*O*-palmitoyl-sn-glycerol (6b)

¹H NMR

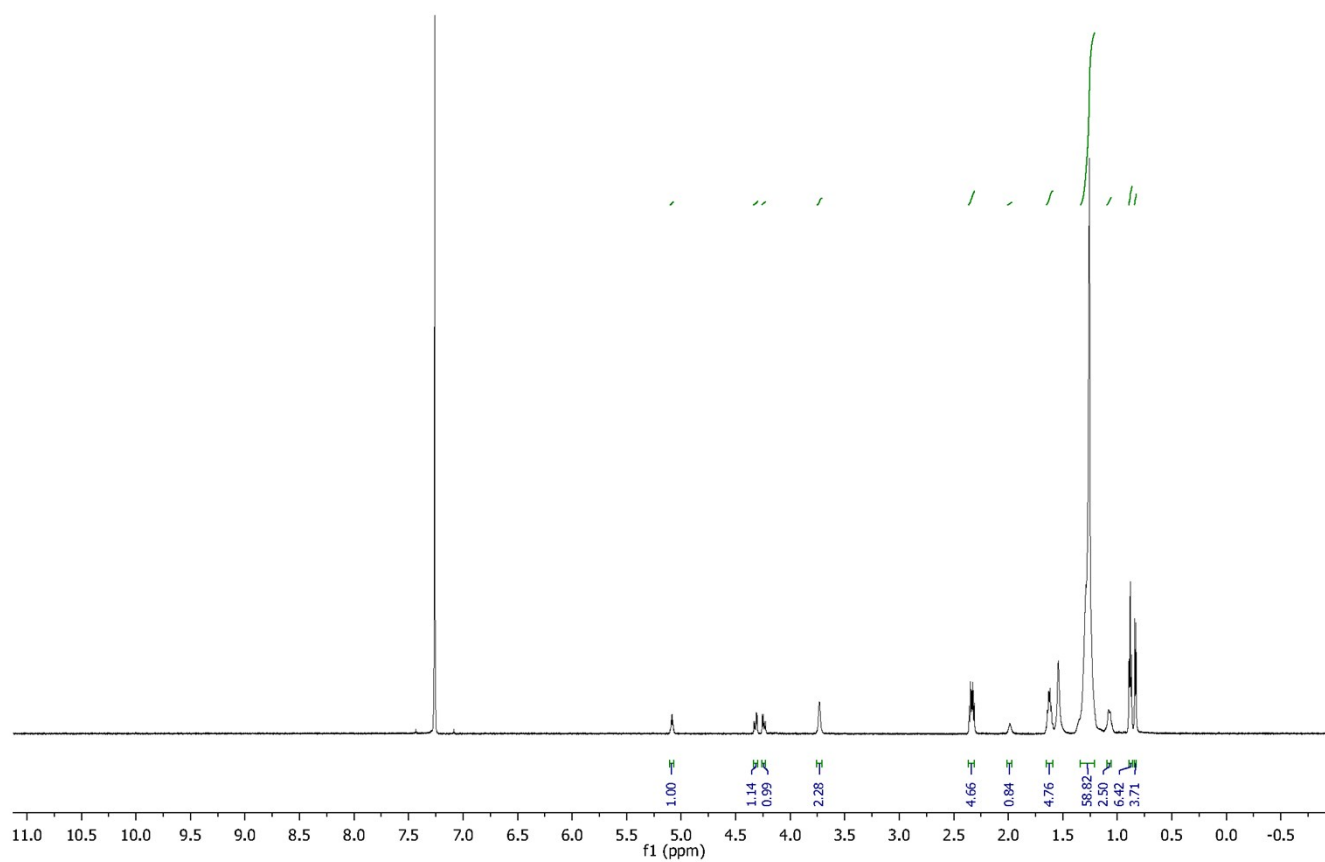


¹³C NMR



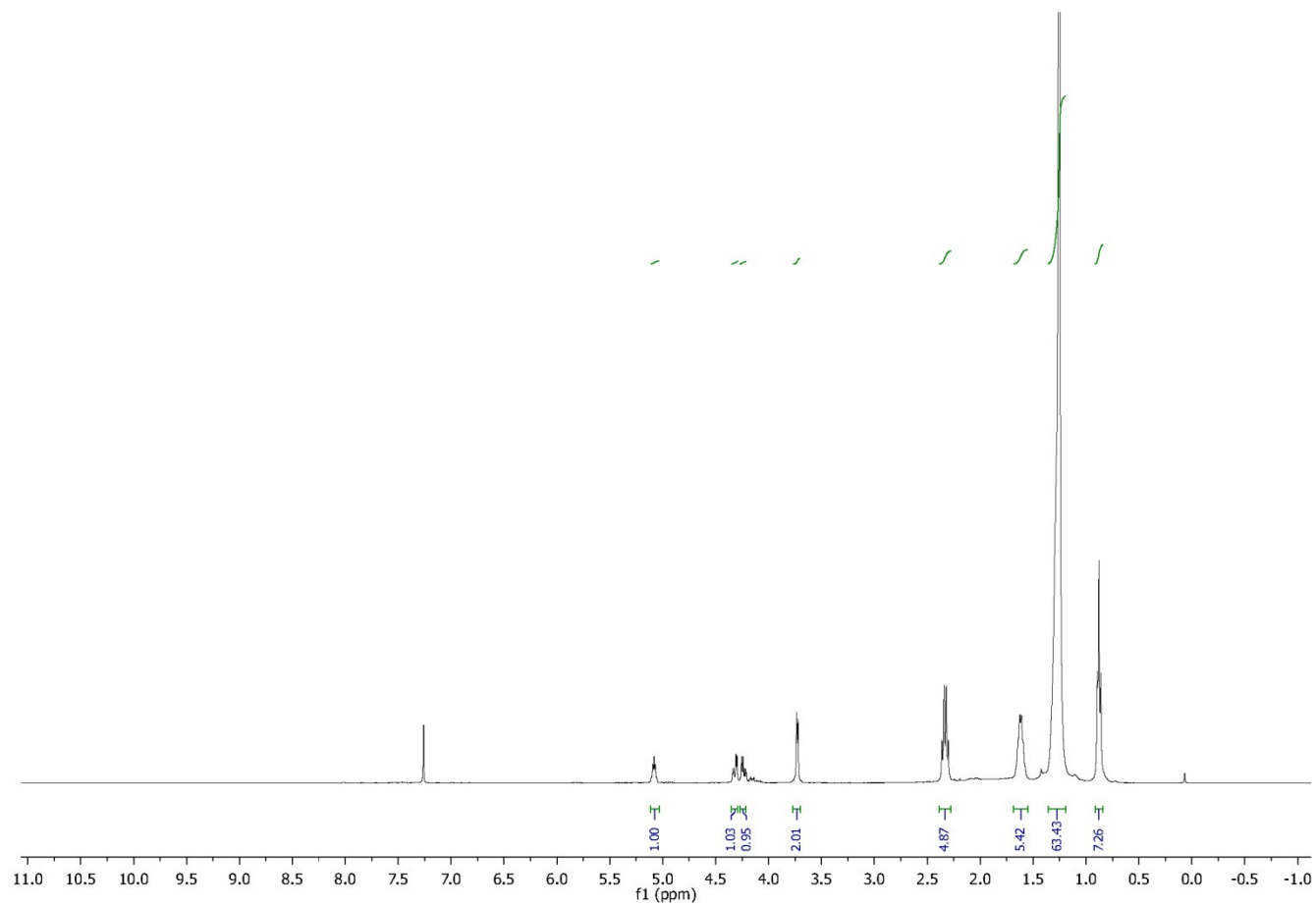
1-*O*-((*R*)-10-Methyloctadecanoyl)-2-*O*-palmitoyl-sn-glycerol (7c)

¹H NMR



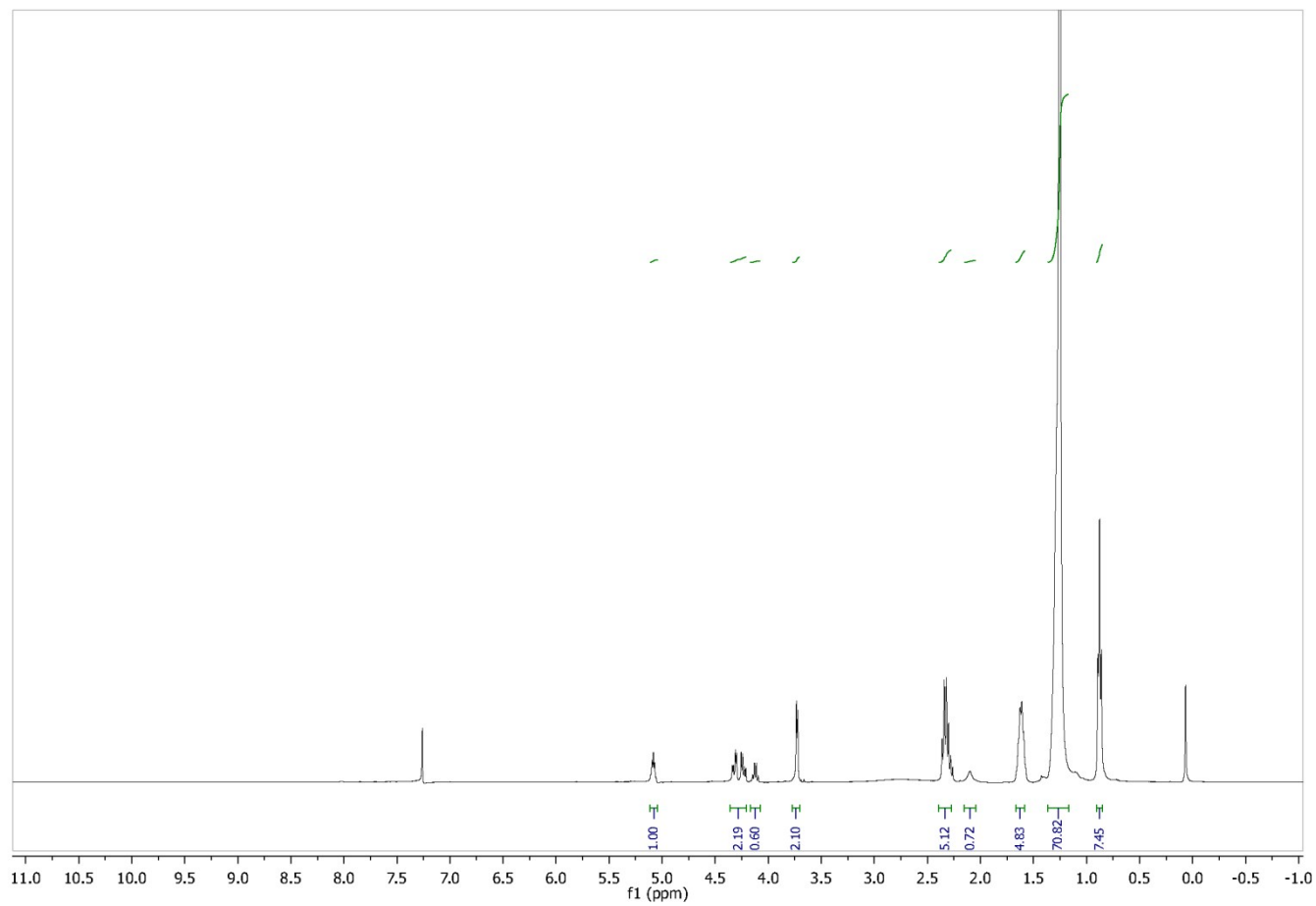
1-*O*-Palmitoyl-2-*O*-stearoyl-sn-glycerol (7a)

¹H NMR



1-*O*-Stearoyl-2-*O*-palmitoyl-sn-glycerol (7b)

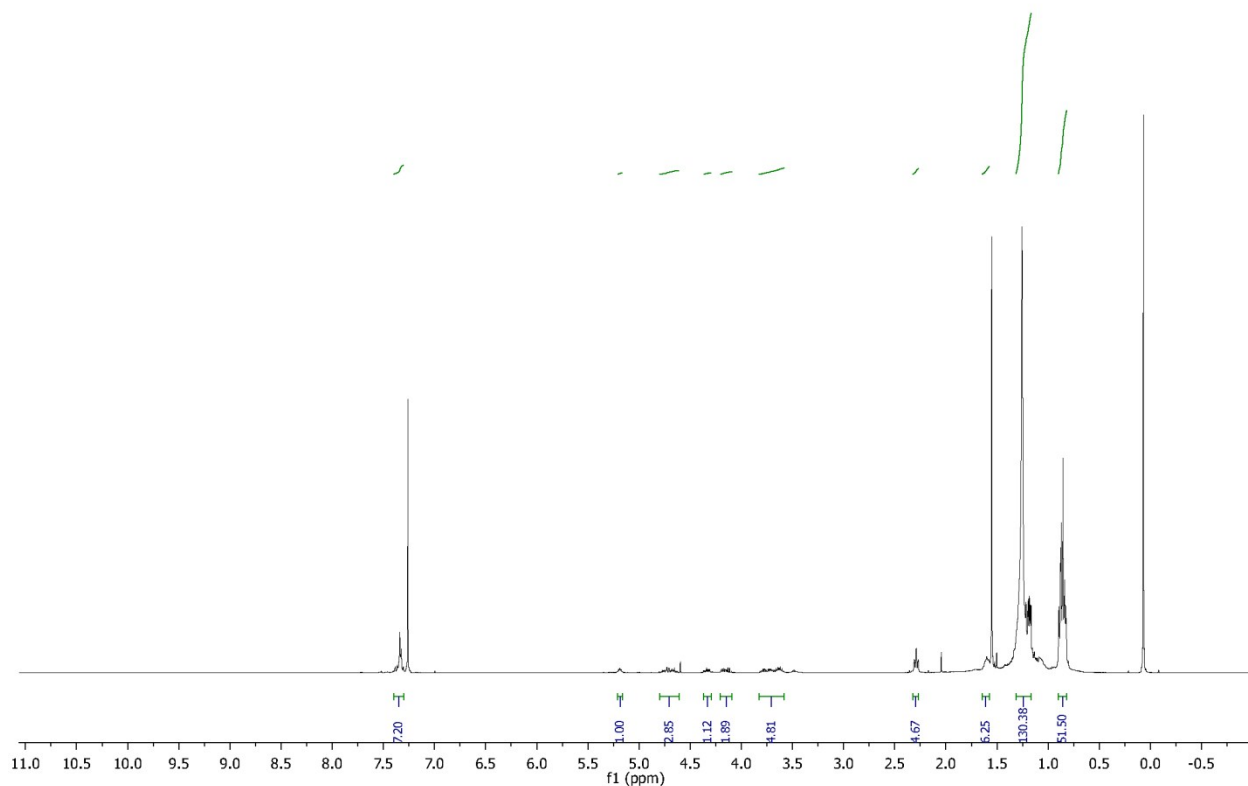
¹H NMR



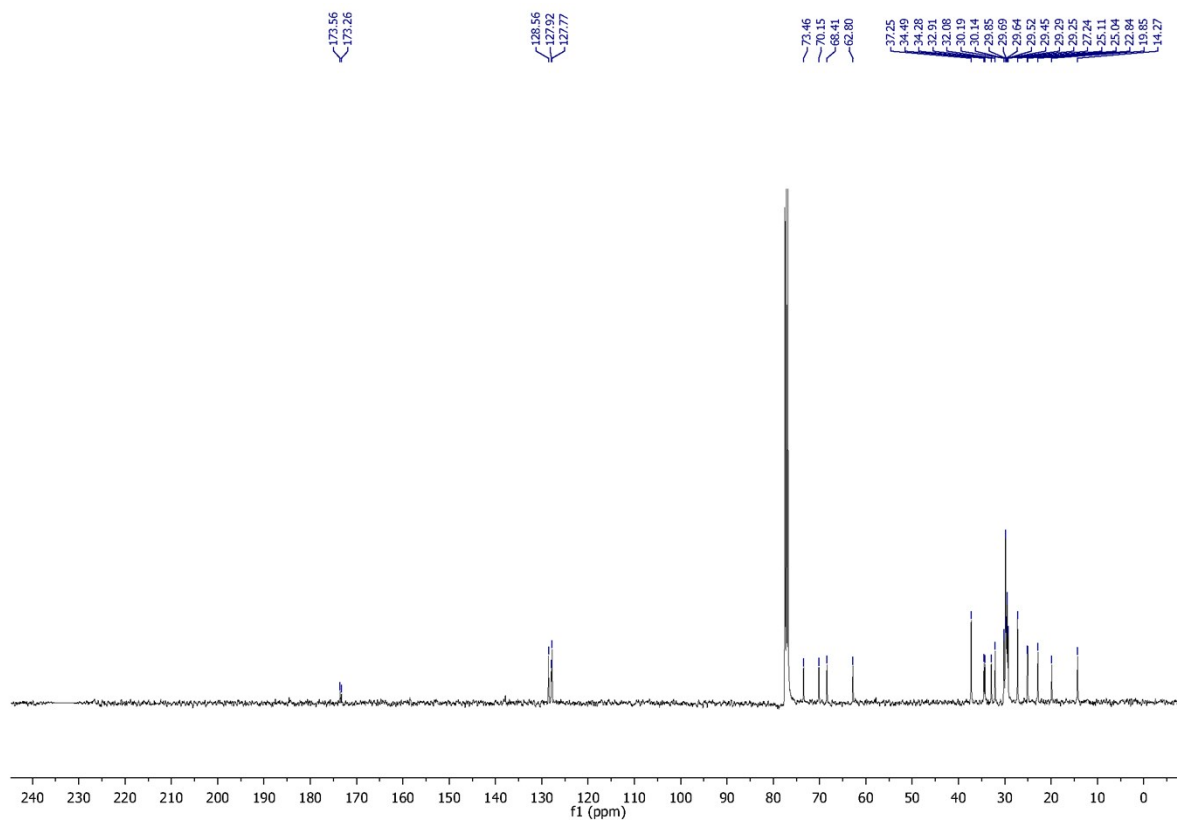
***O*-Benzyl-*O*-(1-*O*-((*R*)-10-methyloctadecanoyl)-2-*O*-palmitoyl-*sn*-glycer-3-yl)
diisopropylphosphoramidite (8c)**

N,N-

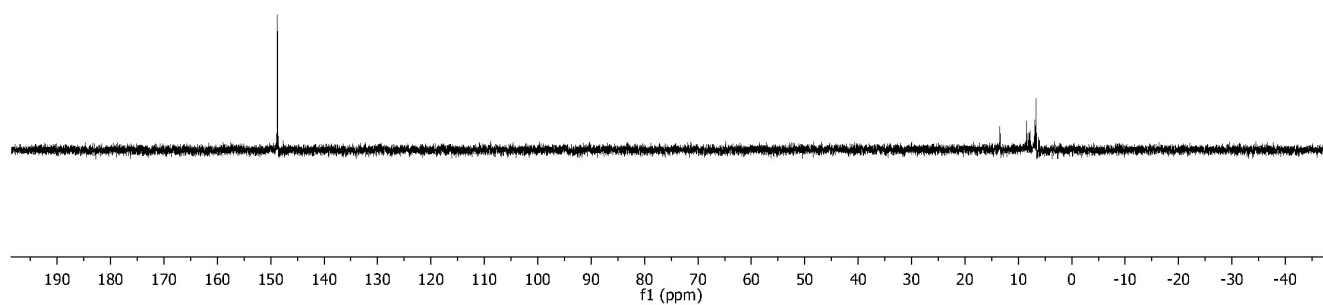
¹H NMR



¹³C NMR

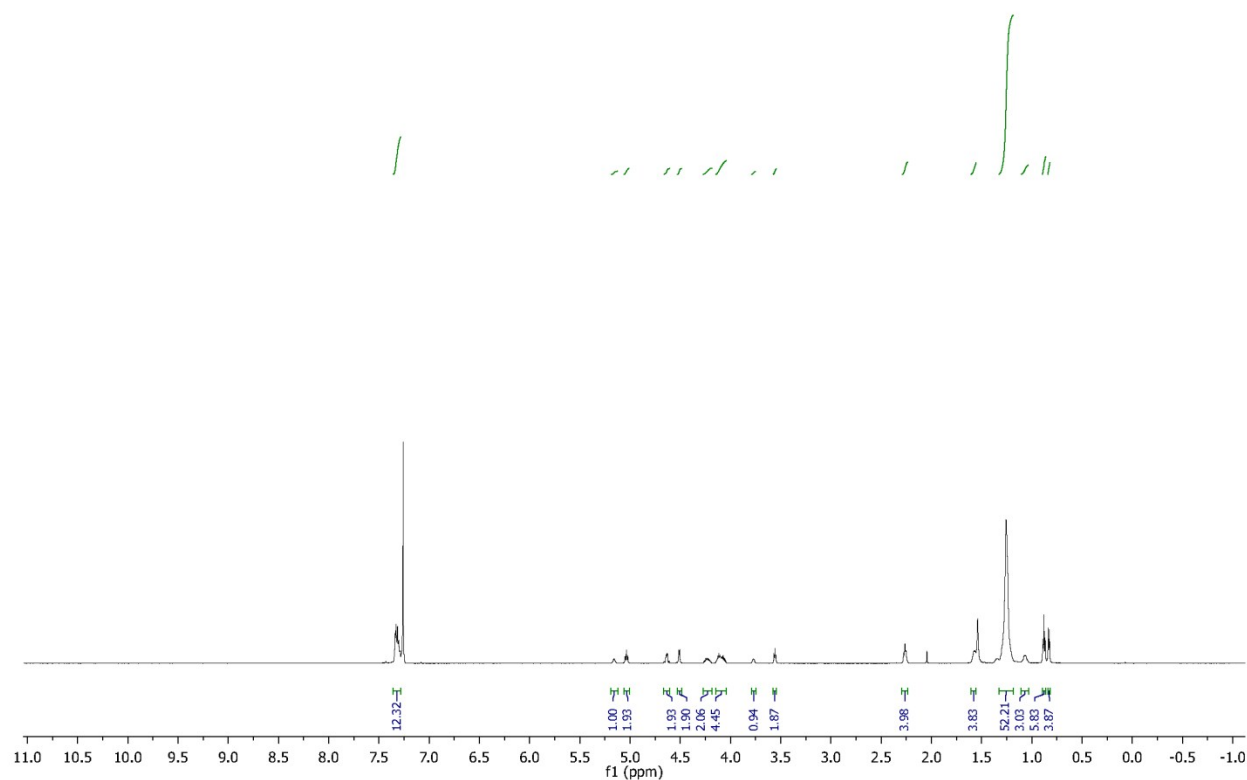


^{31}P NMR

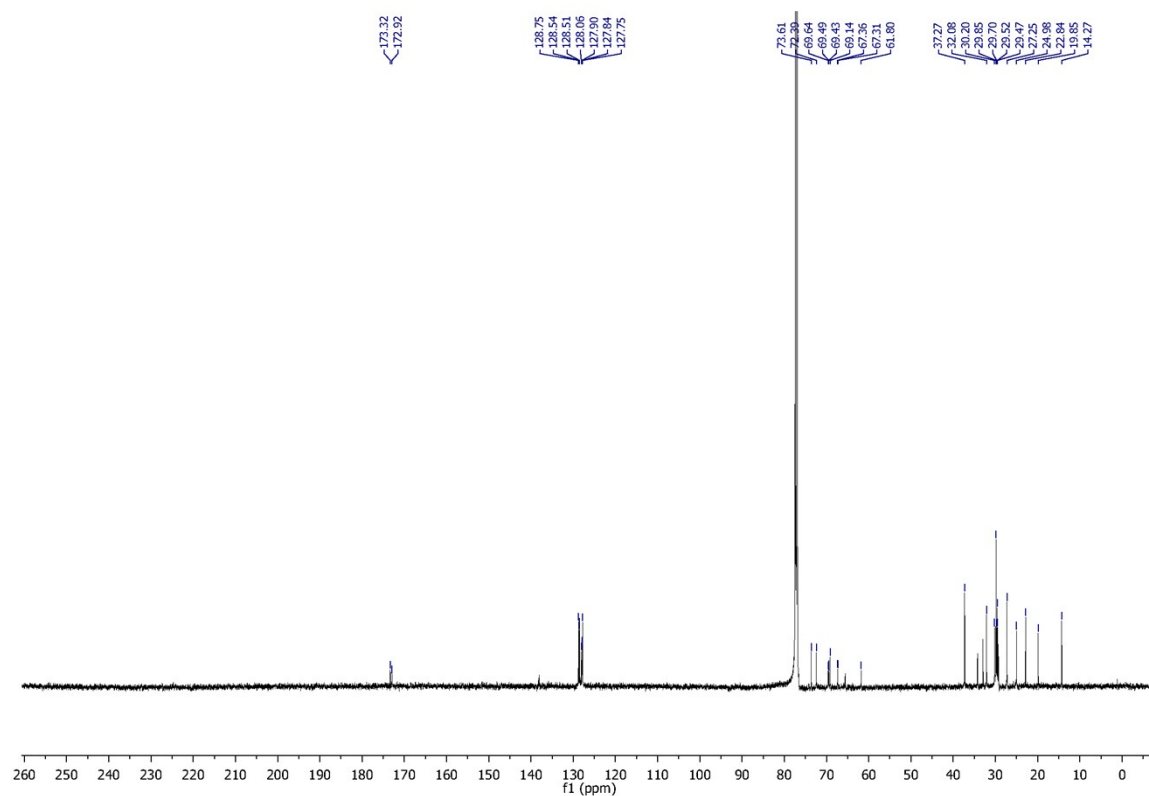


***O*-Benzyl-*O*-(1-*O*-((*R*)-10-methyloctadecanoyl)-2-*O*-palmitoyl-sn-glycerol)-*O*-(2,3-di-*O*-benzyl-sn-glycerol-1-yl) phosphate (10c)**

¹H NMR

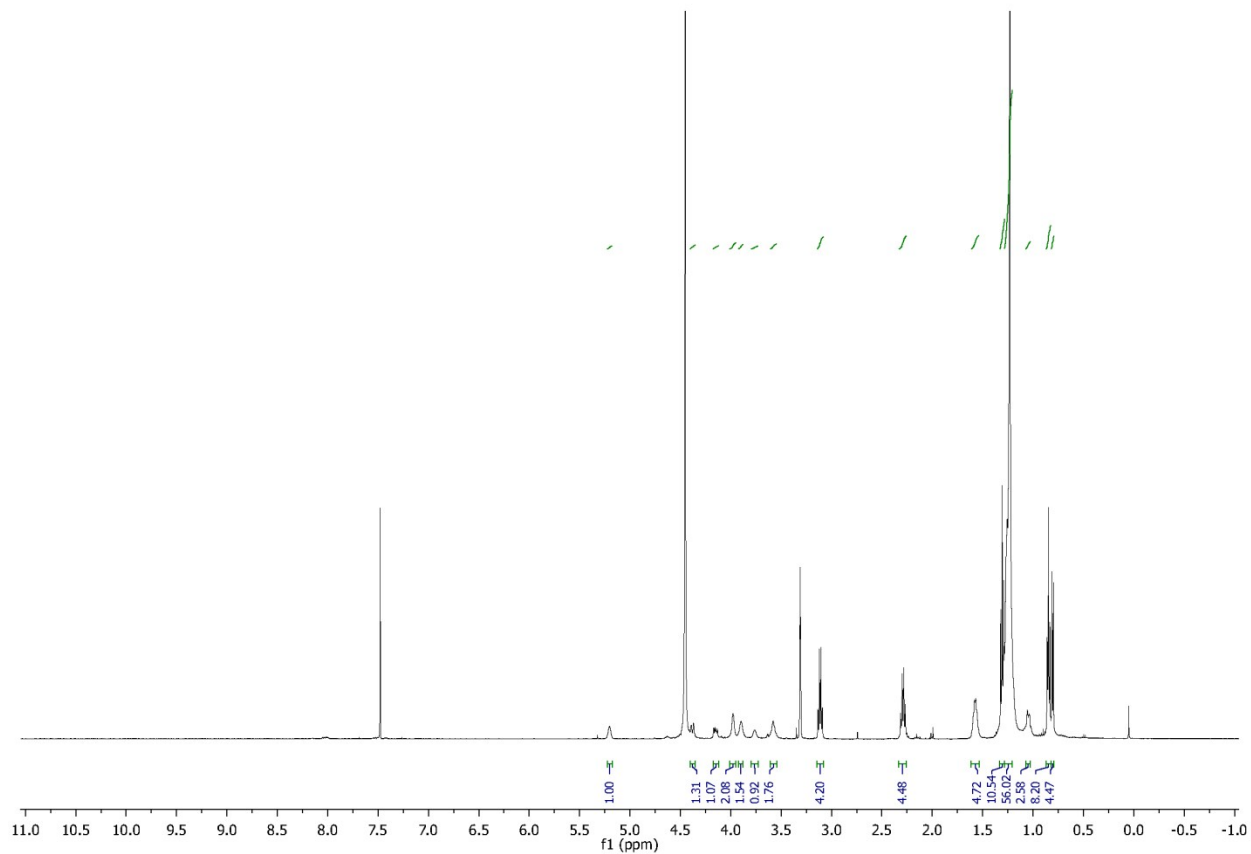


¹³C NMR

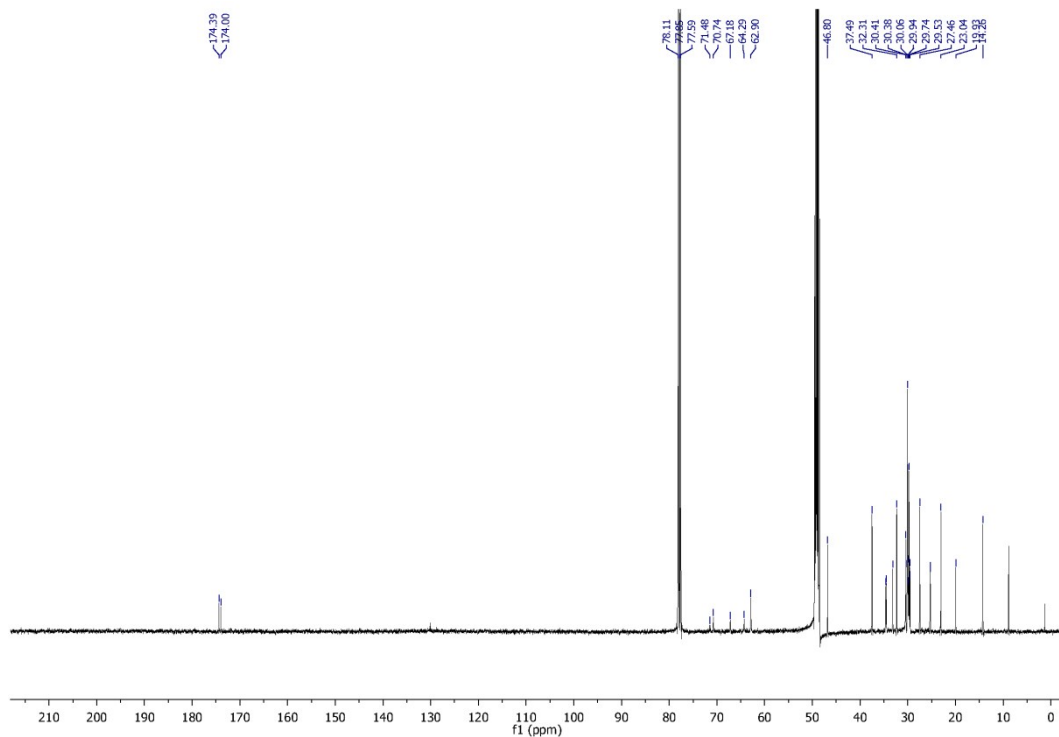


Triethylammonium *O*-(1-*O*-(*R*)-10-methyloctadecanoyl-2-*O*-palmitoyl-sn-glycerol)-*O*-(sn-glycer-1-yl) phosphate (1)

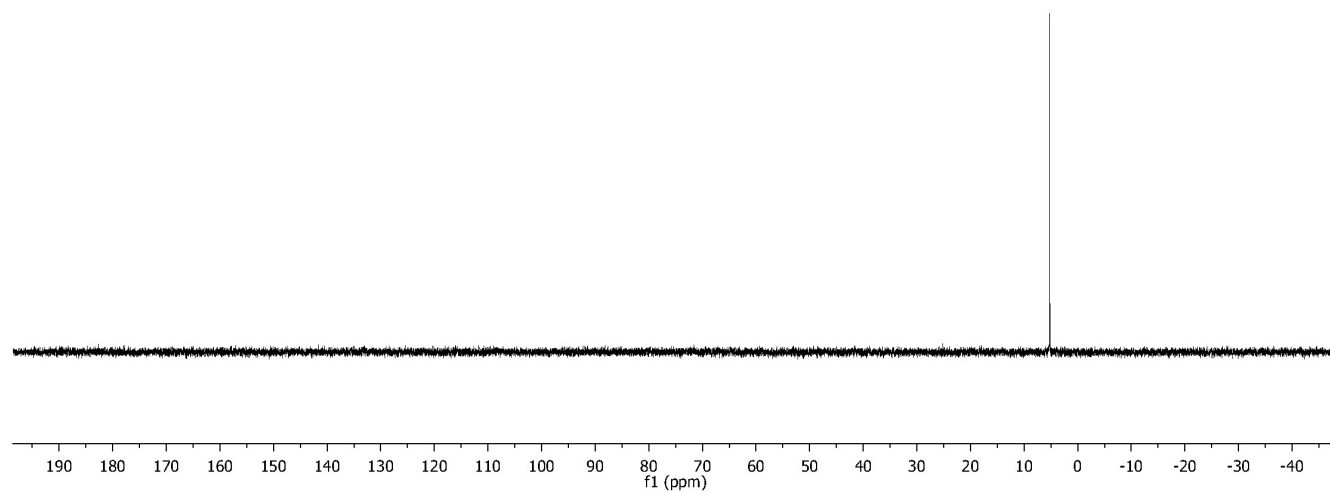
¹H NMR



¹³C NMR

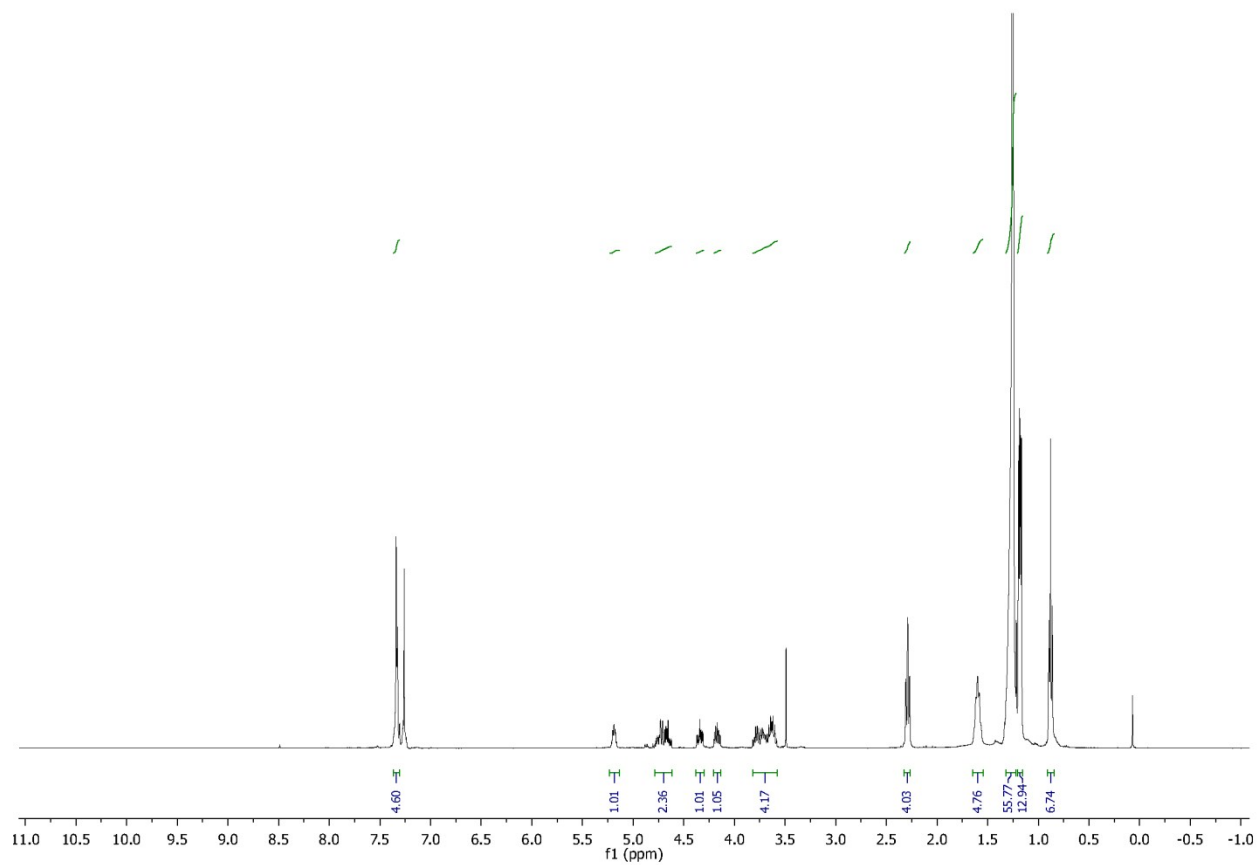


^{31}P NMR

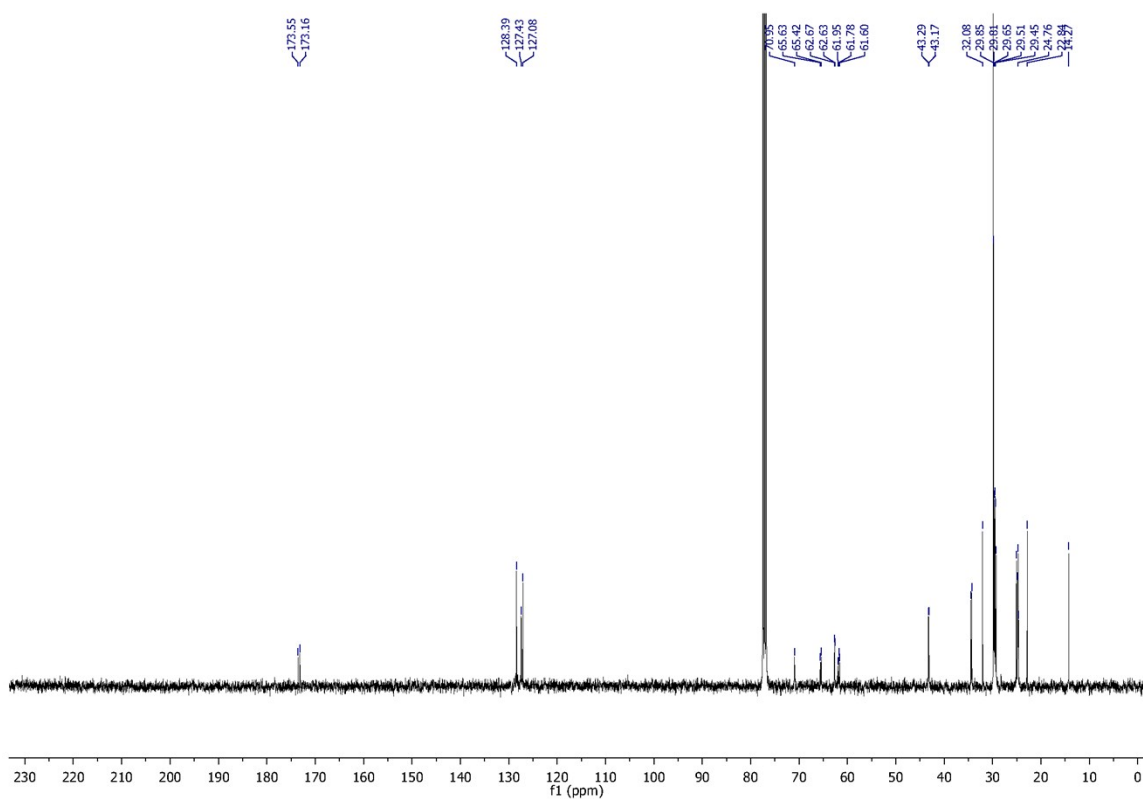


***O*-Benzyl-*O*-(1-*O*-(palmitoyl)-2-*O*-stearoyl-*sn*-glycer-3-yl) *N,N*-diisopropylphosphoramidite (8a)**

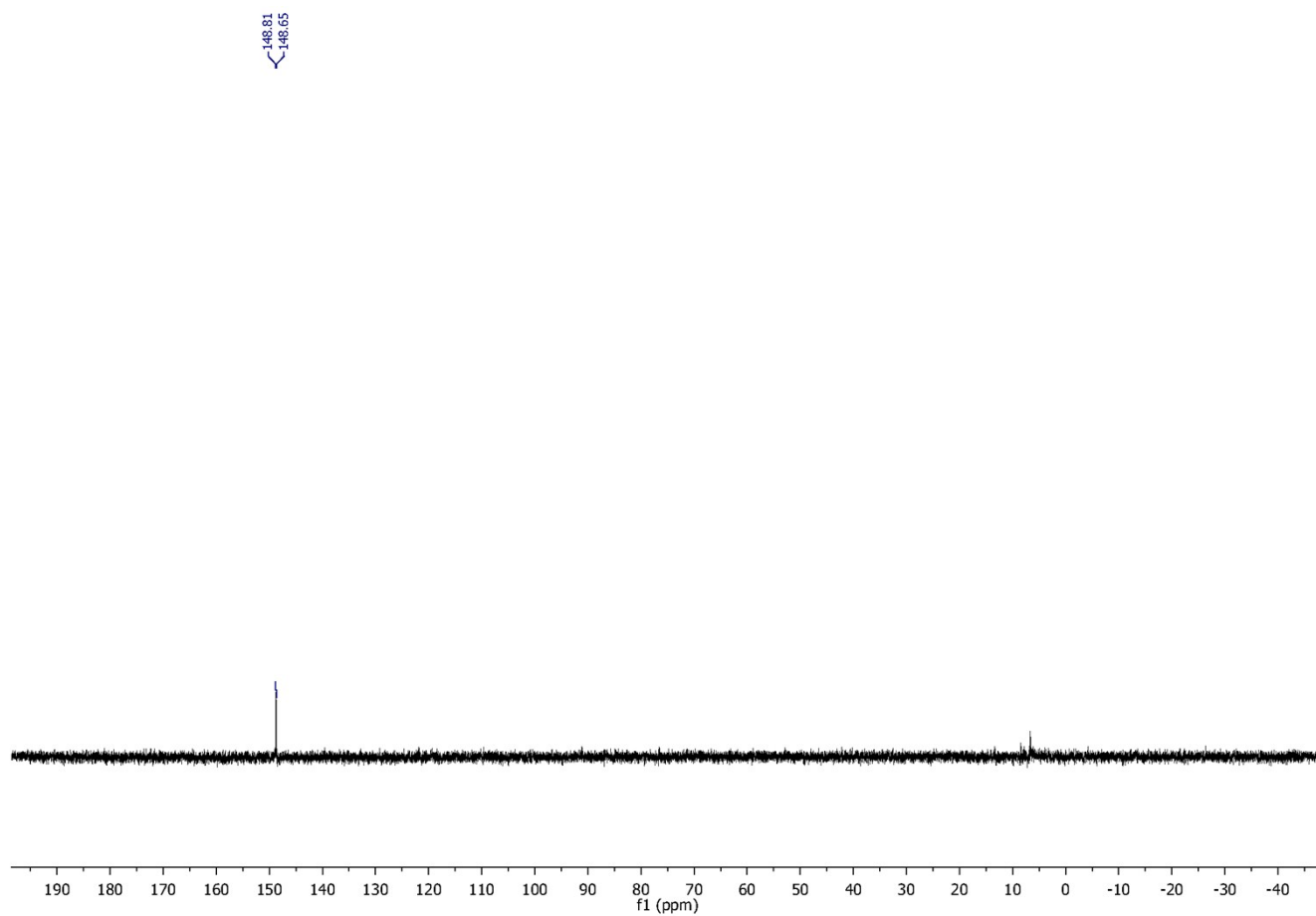
¹H NMR



¹³C NMR

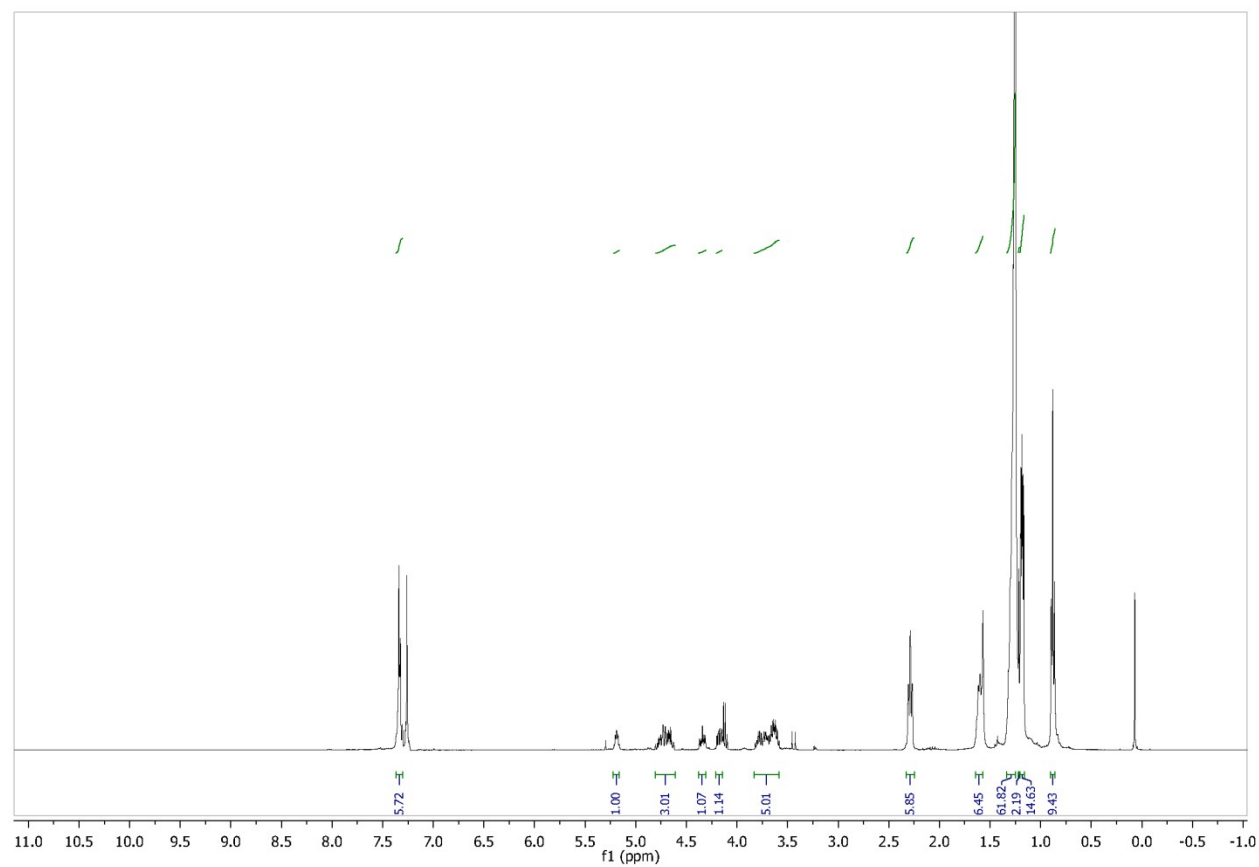


^{31}P NMR

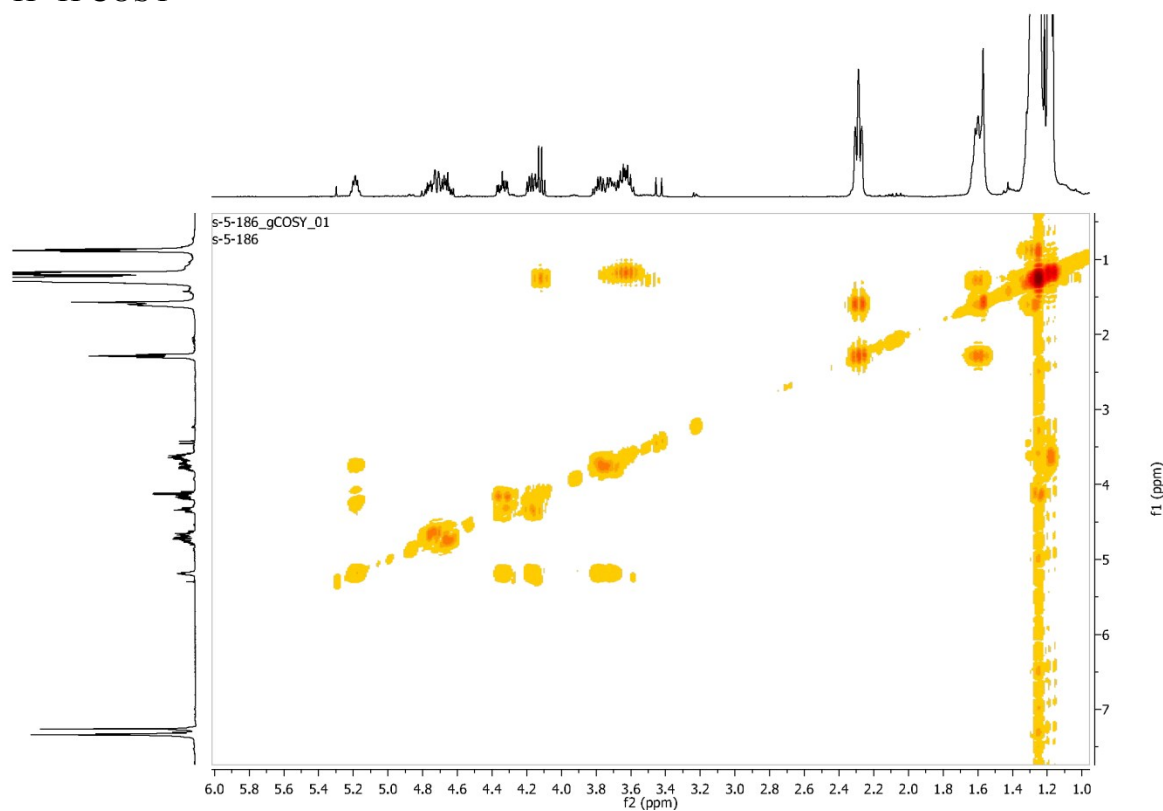


***O*-Benzyl-*O*-(1-*O*-(stearoyl)-2-*O*-palmitoyl-sn-glycer-3-yl) *N,N*-diisopropylphosphoramidite (8b)**

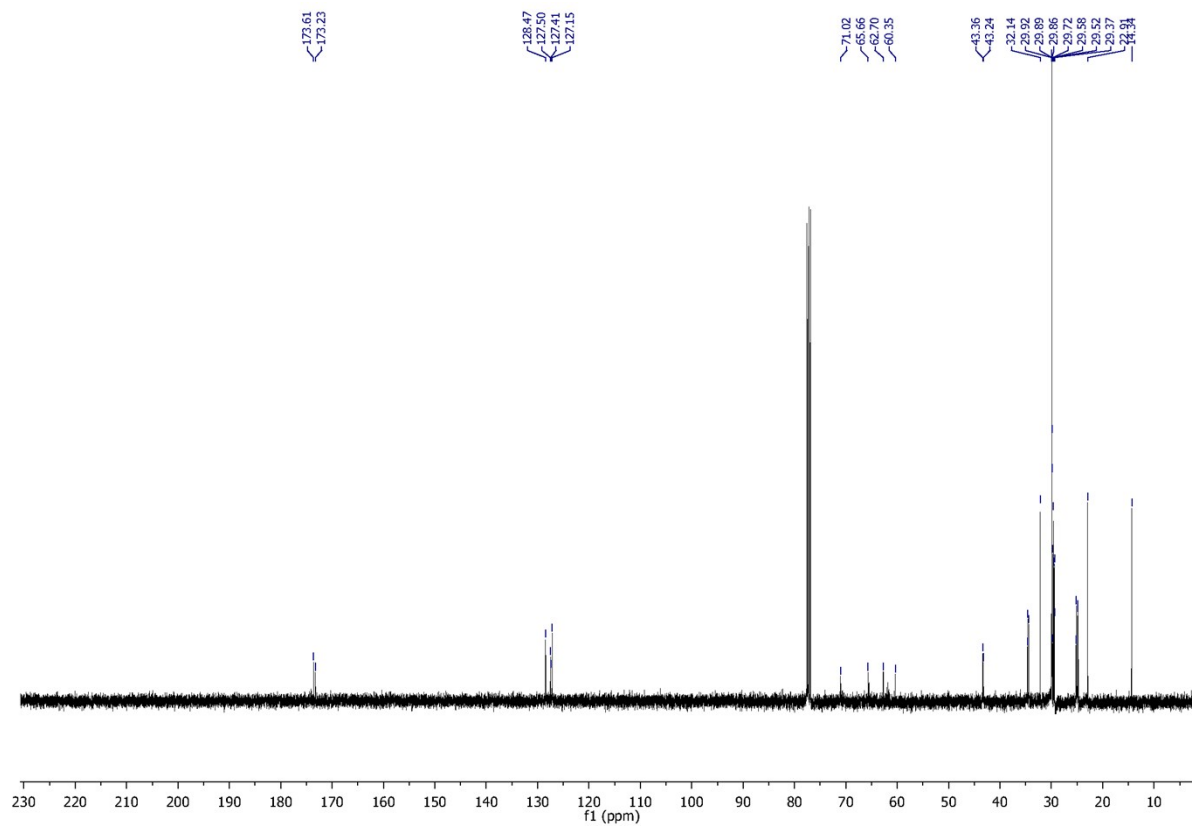
¹H NMR



¹H-¹H COSY

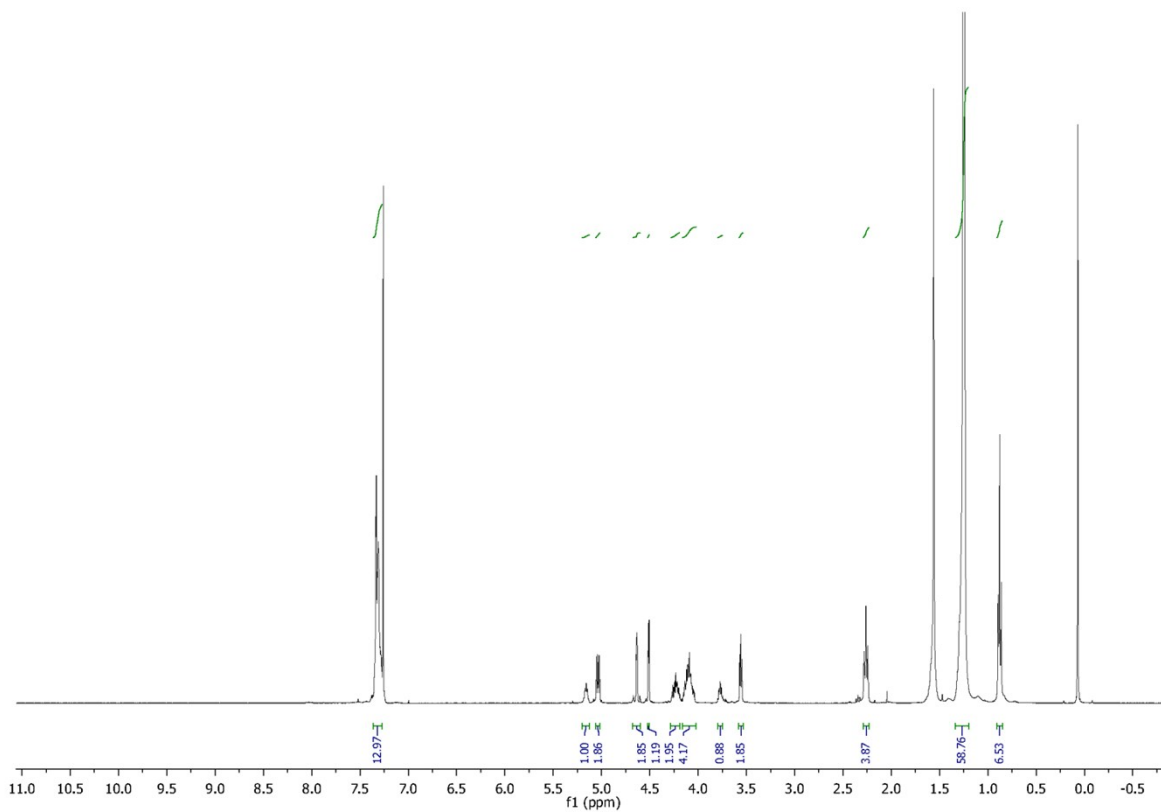


^{13}C NMR

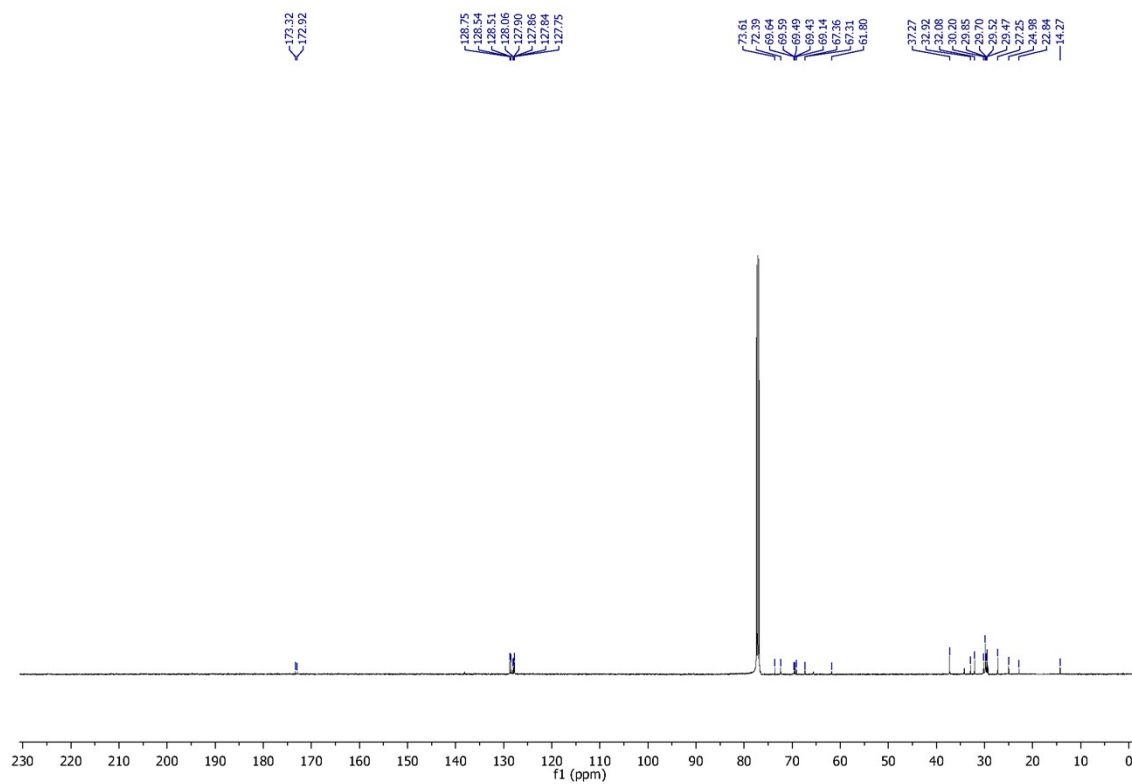


***O*-Benzyl-*O*-(1-*O*-(stearoyl)-2-*O*-palmitoyl-sn-glycer-3-yl)-*O*-(2,3-di-*O*-benzyl-sn-glycer-1-yl) phosphate (10b)**

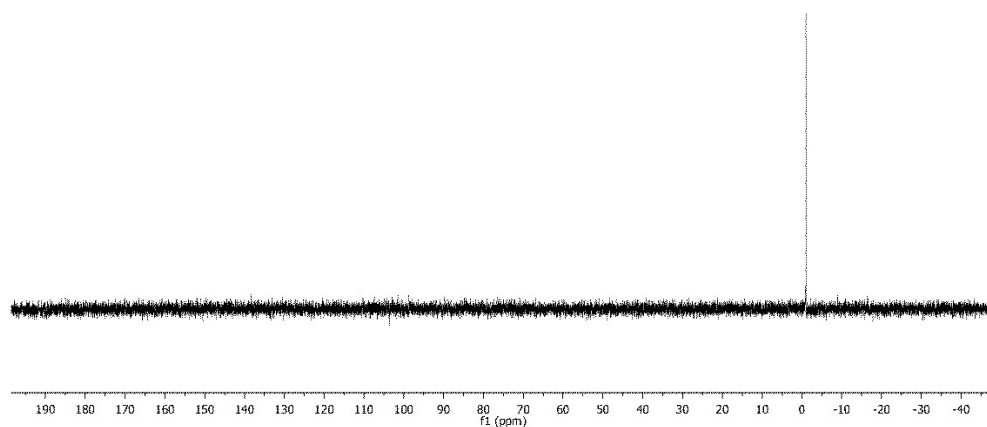
^1H NMR



^{13}C NMR

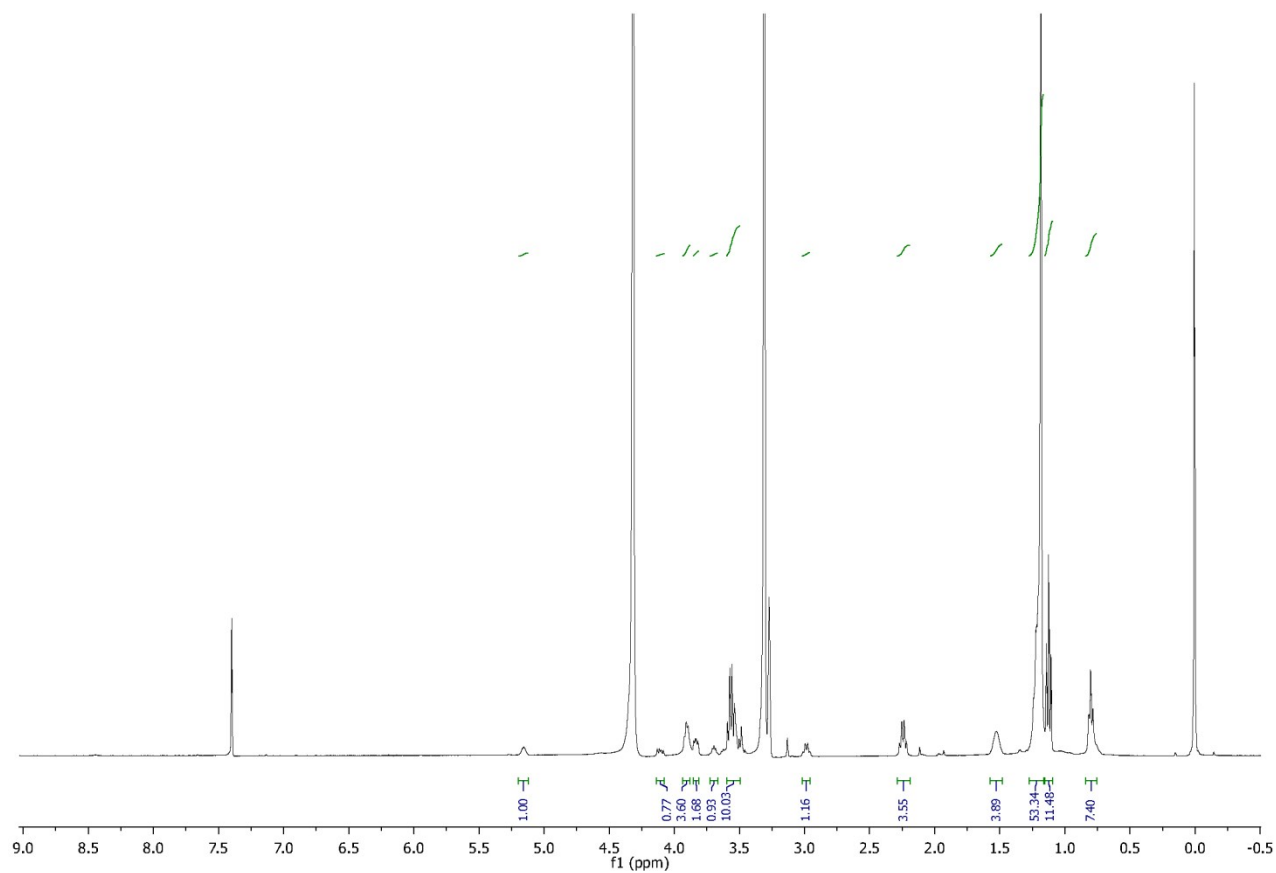


^{31}P NMR

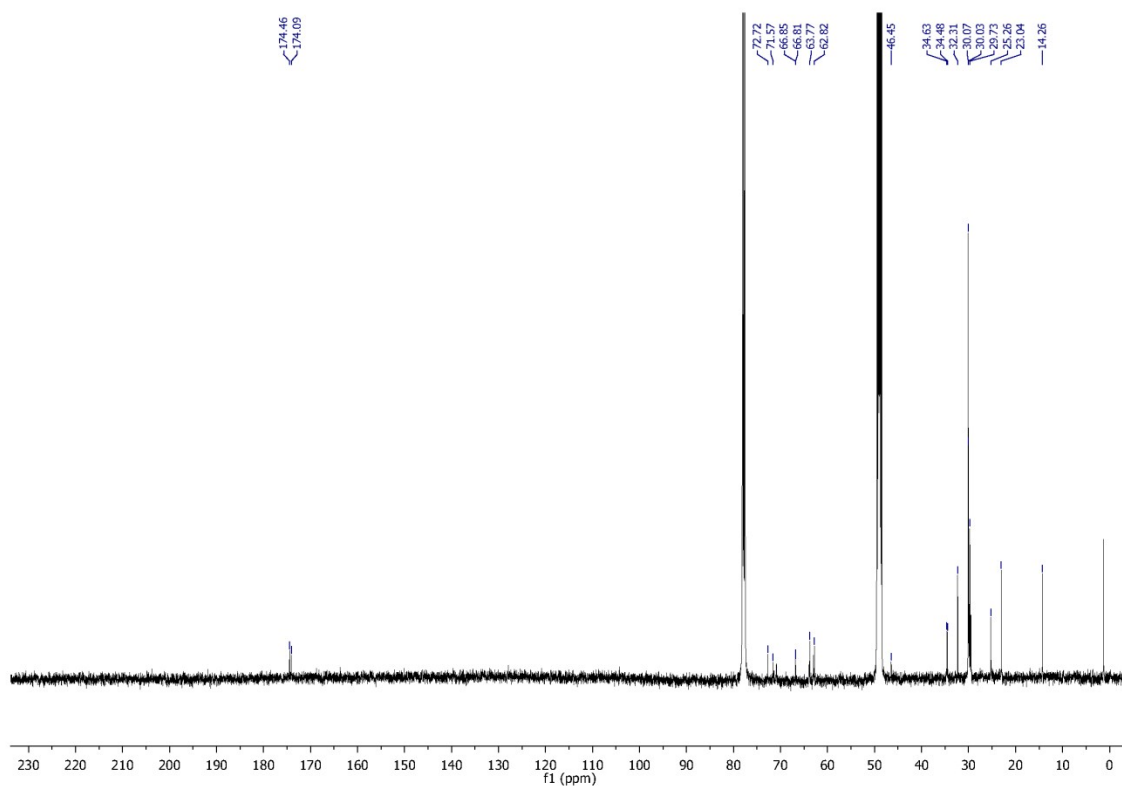


Triethylammonium *O*-(1-*O*-palmitoyl-2-*O*-stearoyl-sn-glycerol)-*O*-(sn-glycer-1-yl) phosphate (11a)

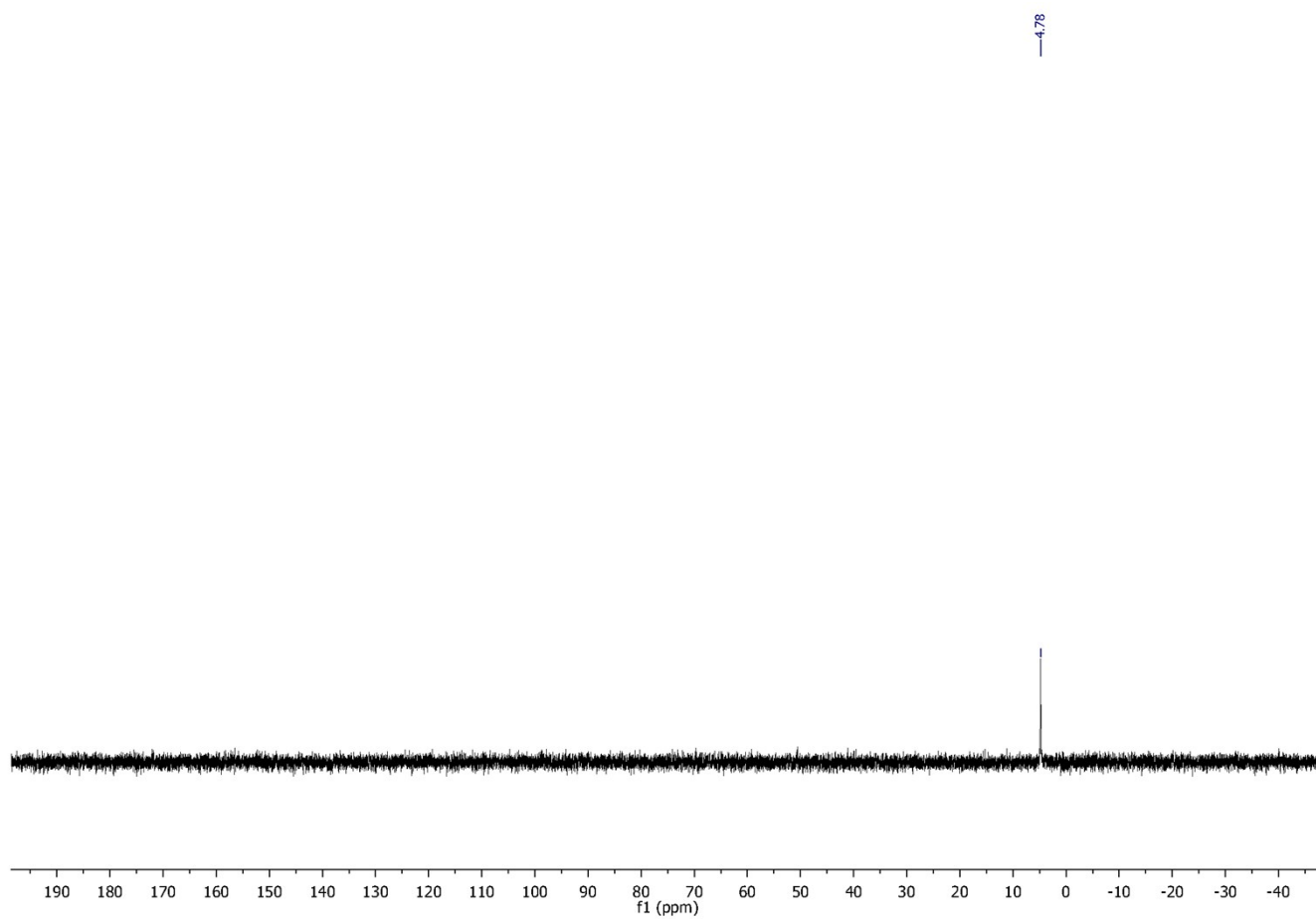
¹H NMR



¹³C NMR

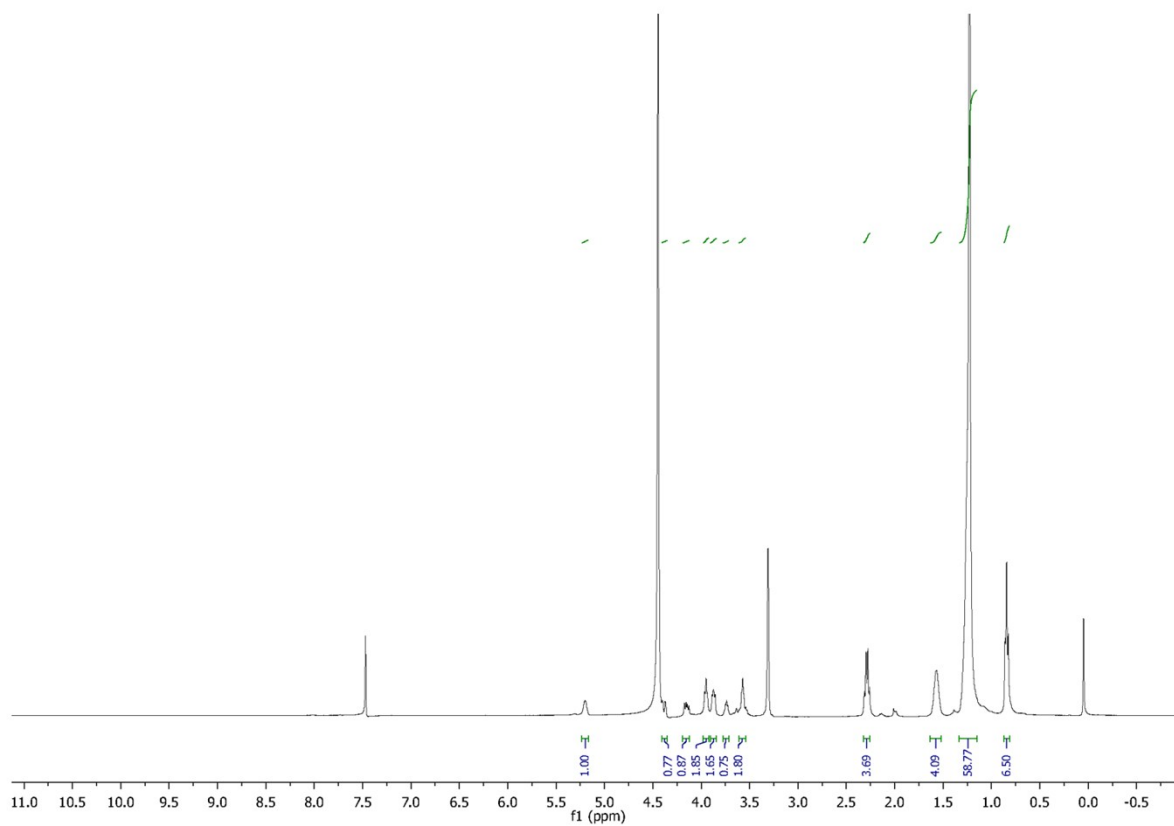


^{31}P NMR

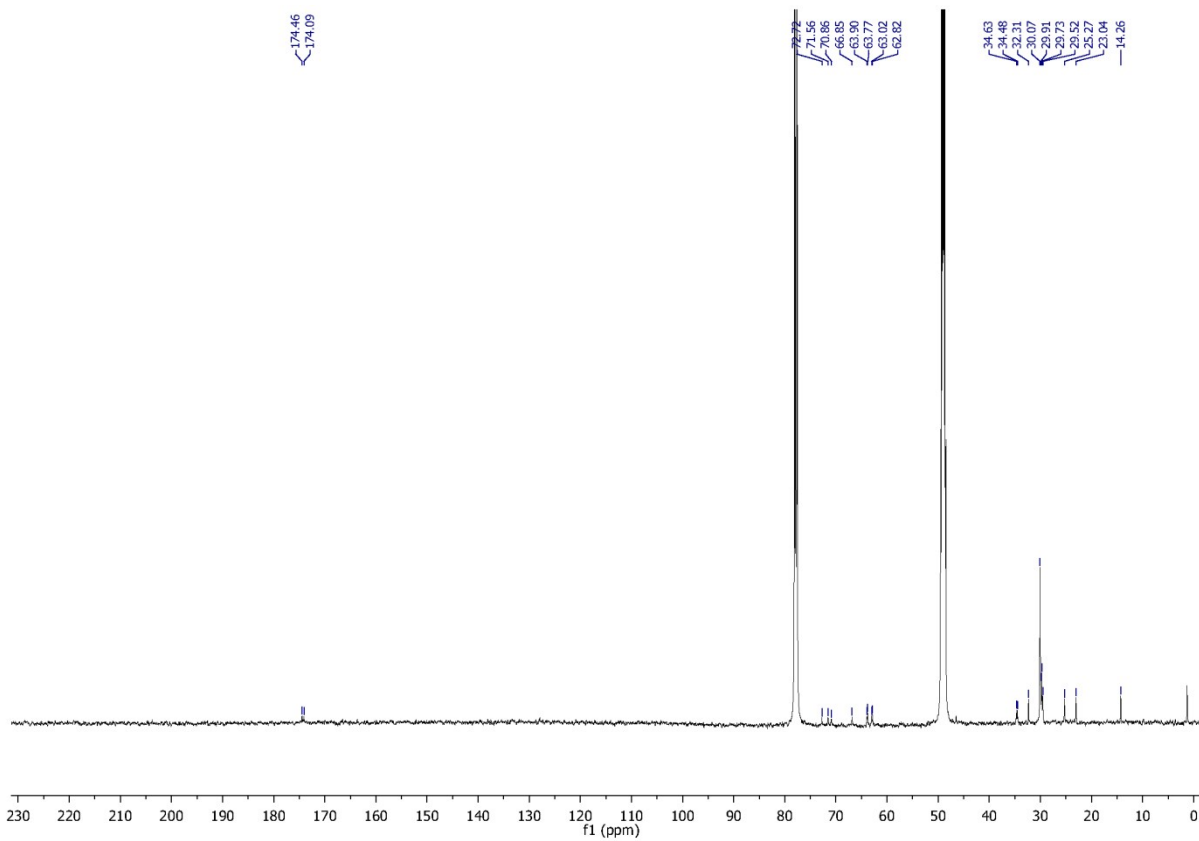


***O*-(1-*O*-Stearoyl-2-*O*-palmitoyl-sn-glyceryl)-*O*-(sn-glycer-1-yl) phosphate (11b)**

¹H NMR



¹³C NMR



^{31}P NMR

