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

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

$^{13}$C NMR
Ethyl (R)-10-methyloctadecanoate

$^1$H NMR

$^{13}$C NMR
(R)-10-Methyloctadecanoic acid (2)

$^1$H NMR

$^{13}$C NMR
3-\textit{O}-Benzyl-1-\textit{O}-(\textit{R})-10-methyloctadecanoyl)-2-\textit{O}-palmitoyl-sn-glycerol (6c)

$^1$H NMR

$^{13}$C NMR
3-O-Benzyl-1-O-palmitoyl-2-O-stearoyl-sn-glycerol (6a)

$^1$H NMR

$^{13}$C NMR
3-O-Benzyl-1-O-stearoyl-2-O-palmitoyl-sn-glycerol (6b)

$^1$H NMR

$^{13}$C NMR
1-O-((R)-10-Methyloctadecanoyl)-2-O-palmitoyl-sn-glycerol (7c)

$^1$H NMR
1-O-Palmitoyl-2-O-stearoyl-sn-glycerol (7a)

$^1$H NMR
1-O-Stearoyl-2-O-palmitoyl-sn-glycerol (7b)

$^1$H NMR
O-Benzyl-O-(1-O-((R)-10-methylhexadecanoyl)-2-O-palmitoyl-sn-glycer-3-yl) \( N,N \)-diisopropylphosphoramidite (8c)

\(^1\)H NMR

\[^{13}\text{C} \) NMR
$^{31}$P NMR
O-Benzyl-\(O\-((R)-10\text{-methyl}10\text{-decenoyl})-2-O\text{-palmitoyl-sn-glyceryl})\-O\-(2,3-di-O\text{-benzyl-sn-glycer-1-yl}) \text{ phosphate (10c)}\)

\(^{1}H \text{ NMR}

\(^{13}C \text{ NMR}

13
Triethylammonium $O$-$1$-$O$-$\text{(R)}$-$10$-$\text{methyloctadecanoyl}$-$2$-$\text{O}$-$\text{palmitoyl}$-$\text{sn}$-$\text{glyceryl}$-$\text{O}$-$\text{sn}$-$\text{glycer}$-$1$-$\text{yl}$ phosphate (1)

$^1$H NMR

$^{13}$C NMR
$^{31}$P NMR
O-Benzyl-O-(1-O-(palmitoyl)-2-O-stearoyl-sn-glycer-3-yl) N,N-diisopropylphosphoramide (8a)

$^1$H NMR

$^{13}$C NMR
$^{31}$P NMR
$O$-Benzyl-$O$-(1-$O$-(stearoyl)-2-$O$-palmitoyl-sn-glycer-3-yl) $N,N$-diisopropylphosphoramidite (8b)

$^1$H NMR

$^1$H-$^1$H 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)

$^1$H NMR

$^{13}$C NMR
Triethylammonium $O$-(1-$O$-palmitoyl-2-$O$-stearoyl-sn-glyceryl)-$O$-(sn-glycer-1-yl) phosphate (11a)

$^1$H NMR

$^{13}$C NMR
O-(1-O-Stearoyl-2-O-palmitoyl-sn-glyceryl)-O-(sn-glycer-1-yl) phosphate (11b)

$^1$H NMR

$^{13}$C NMR
$^{31}$P NMR