Supporting Information

for

A practical synthesis of long-chain iso-fatty acids

(iso-C_{12}–C_{19}) and related natural products

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NMR spectra

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$^1$H NMR (500 MHz, CDCl$_3$) – 10-Methylundecanoic acid (I)

![Carbon-13 NMR spectrum of 10-Methylundecanoic acid (I)](image)

CDCl$_3$
$^{13}$C NMR (125 MHz, CDCl$_3$) – 10-Methylundecanoic acid (I)
$^1$H NMR (500 MHz, CDCl$_3$) – 11-Methyldodecanoic acid (2)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 11-Methyldodecanoic acid (2)
$^1$H NMR (500 MHz, CDCl$_3$) – 12-Methyltridecanoic acid (3)
$\text{C NMR (125 MHz, CDCl}_3\text{)}$ – 12-Methyltridecanoic acid (3)
$^1$H NMR (500 MHz, CDCl$_3$) – 13-Methyltetradecanoic acid (4)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 13-Methyltetradecanoic acid (4)
$^1$H NMR (500 MHz, CDCl$_3$) – 14-Methylpentadecanoic acid (5)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 14-Methylpentadecanoic acid (5)

![14-Methylpentadecanoic acid (5)](image)

CDCl$_3$
$^1$H NMR (500 MHz, CDCl$_3$) – 15-Methylhexadecanoic acid (6)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 15-Methylhexadecanoic acid (6)
\(^1\)H NMR (500 MHz, CDCl\(_3\)) – 16-Methylheptadecanoic acid (7)
$\text{C NMR (125 MHz, CDCl}_3\text{) – 16-Methylheptadecanoic acid (7)}$
$^1$H NMR (500 MHz, CDCl$_3$) – 17-Methyloctadecanoic acid (8)

\[
\text{CO}_2\text{H} \\
\text{15}
\]

CDCl$_3$
$^{13}$C NMR (125 MHz, CDCl$_3$) – 17-Methyloctadecanoic acid (8)
$^{1}\text{H NMR (500 MHz, CDCl}_3\text{)}$ – 2-Methyldodec-11-en-2-ol (10)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 2-Methyldodec-11-en-2-ol (10)
$^1$H NMR (500 MHz, CDCl$_3$) – 11-Methyldodec-1-ene (11)
$^{13}\text{C}$ NMR (125 MHz, CDCl$_3$) – 11-Methyldodec-1-ene (II)
$^1$H NMR (500 MHz, CDCl$_3$) – 11-Methyldodecan-1-ol (12)

![NMR spectrum of 11-Methyldodecan-1-ol (12)](image-url)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 11-Methyldodecan-1-ol (12)
$^1$H NMR (500 MHz, CDCl$_3$) – 11-Methyldodecyl methanesulfonate (13)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 11-Methyldodecyl methanesulfonate (13)
$^1$H NMR (500 MHz, CDCl$_3$) – 12-Methyltridecanitrile (14)
$^{13}\text{C NMR (125 MHz, CDCl}_3\text{)}$ – 12-Methyltridecanitrile (14)

\[\text{CH}_2\text{CN} \quad \text{CDCl}_3\]
$^1$H NMR (500 MHz, DMSO-$d_6$) – 15-Methylhexadecane-1,15-diol (16)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 15-Methylhexadecane-1,15-diol (16)

![C NMR spectrum of 15-Methylhexadecane-1,15-diol (16)](image)

CDCl$_3$
$^1$H NMR (500 MHz, CDCl$_3$) – 15-Methylhexadecan-1-ol (17)

CDCl$_3$
$^{13}$C NMR (125 MHz, CDCl$_3$) – 15-Methylhexadecan-1-ol (17)
$^1$H NMR (500 MHz, CDCl$_3$) – S-Methyl-O-15-methylhexadecyl dithiocarbonate (18)
$^{13}$C NMR (125 MHz, CDCl$_3$) – S-Methyl-O-15-methylhexadecyl dithiocarbonate (18)
$^1$H NMR (500 MHz, CDCl$_3$) – 15-Methylhexadecan-1-ene (19)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 15-Methylhexadecan-1-ene (19)
$^1$H NMR (500 MHz, CDCl$_3$) – 14-Methylpentadecan-1-ol (20)

\[ \text{CH}_2\text{OH} \]

CDCl$_3$
$^{13}$C NMR (125 MHz, CDCl$_3$) – 14-Methylpentadecan-1-ol (20)
$^1$H NMR (500 MHz, CDCl$_3$) – 14-Methylpentadec-1-ene (22)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 14-Methylpentadec-1-ene (22)
\(^1\)H NMR (500 MHz, DMSO-\(d_6\)) – 16-Methylheptadecane-1,16-diol (24)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 16-Methylheptadecane-1,16-diol (24)
$^1$H NMR (500 MHz, CDCl$_3$) – 16-Methylheptadecan-1-ol (25)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 16-Methylheptadecan-1-ol (25)

\[
\begin{align*}
\text{CH}_2\text{OH} \\
\text{CDCl}_3
\end{align*}
\]
$^1$H NMR (500 MHz, CDCl$_3$) – 16-Methylheptadecyl methanesulfonate (26)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 16-Methylheptadecyl methanesulfonate (26)
$^1$H NMR (500 MHz, CDCl$_3$) – 17-Methyloctadecanenitrile (27)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 17-Methyloctadecanenitrile (27)
$^1$H NMR (500 MHz, CDCl$_3$) – (S)-4-Benzyl-3-(15-methylhexadecanoyl)oxazolidin-2-one (28)
$^{13}$C NMR (125 MHz, CDCl$_3$) – (S)-4-Benzyl-3-(15-methylhexadecanoyl)oxazolidin-2-one (28)
$^{13}$C NMR (125 MHz, CDCl$_3$) – (S)-4-Benzyl-3-((S)-2,15-dimethylhexadecanoyl)oxazolidin-2-one (29)
$^1$H NMR (500 MHz, CDCl$_3$) – (S)-4-Benzyl-3-((S)-2,15-dimethylhexadecanoyl)oxazolidin-2-one (29)
$^1$H NMR (500 MHz, CDCl$_3$) – (S)-2,15-Dimethylhexadecanoic acid (30)
$^{13}$C NMR (125 MHz, CDCl$_3$) – (S)-2,15-Dimethylhexadecanoic acid (30)
$^1$H NMR (500 MHz, CDCl$_3$) – 3-Phenyl-2-(phenylsulfonyl)-1,2-oxaziridine

PhO$_2$S$^-$

Ph

CDCl$_3$

H$_2$O
$^{13}$C NMR (125 MHz, CDCl$_3$) – 3-Phenyl-2-(phenylsulfonyl)-1,2-oxaziridine

![Chemical Structure]
$^1$H NMR (500 MHz, CDCl$_3$) – (S)-4-Benzyl-3-((S)-2-hydroxy-15-methylhexadecanoyl)oxazolidin-2-one (31)
$^{13}\text{C NMR (125 MHz, CDCl}_3\text{)}$ – (S)-4-Benzyl-3-((S)-2-hydroxy-15-methylhexadecanoyl)oxazolidin-2-one (31)
$^1$H NMR (500 MHz, CDCl$_3$) – (S)-Methyl 2-hydroxy-15-methylhexadecanoate
$^{13}$C NMR (125 MHz, CDCl$_3$) – (S)-Methyl 2-hydroxy-15-methylhexadecanoate
$^1$H NMR (500 MHz, CDCl$_3$/CD$_3$OD) – (S)-2-Hydroxy-15-methylhexadecanoic acid (32)
$^{13}$C NMR (125 MHz, DMSO-$d_6$/TFA) – (S)-2-Hydroxy-15-methylhexadecanoic acid (32)
$^1$H NMR (500 MHz, CDCl$_3$) – 14-Methylpentadecan-2-one (33)
$^{13}$C NMR (125 MHz, CDCl$_3$) – 14-Methylpentadecan-2-one (33)