Electronic Supplementary Information

Aerobic oxidative esterification and thioesterification of aldehydes using dibromoisocyanuric acid under mild conditions: no metal catalysts required

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Contents

NMR Spectra .................................................................................................................................................. S2-S41
Benzyl benzoate (4a)
Butyl benzoate (4b)
Cyclohexyl benzoate (4c)
Benzhydryl benzoate (4d)

Chemical structure and NMR spectrum of Benzhydryl benzoate (4d). The spectrum shows resonances at various chemical shifts.

X: parts per Million - 1H

X: parts per Million - Carbon13

Abundance values are indicated for different chemical shifts.

S5
Phenyl benzoate (4e)
Benzyl 4-methylbenzoate (4f)

X : parts per Million : Proton

X : parts per Million : Carbon13
4-Nitrobenzyl 4-methylbenzoate (4g)

![NMR spectrum of 4-Nitrobenzyl 4-methylbenzoate](image)

**X**: parts per Million - Proton

**X**: parts per Million - Carbon13
4-Methylbenzyl 4-methylbenzoate (4h)
Prop-2-ynyl 4-methylbenzoate (4i)
Benzyl 4-chlorobenzoate (4j)
4-Nitrobenzyl 4-chlorobenzoate (4k)
4-Methylbenzyl 4-chlorobenzoate (4I)
Cyclohexyl 4-chlorobenzoate (4m)
Butyl 4-chlorobenzoate (4n)

X: parts per Million : 1H

X: parts per Million : 13C
Benzyl 4-nitrobenzoate (4o)
Cyclopropylmethyl 4-nitrobenzoate (4p)
Isobutyl 4-nitrobenzoate (4q)
Allyl 4-nitrobenzoate (4r)
Benzyl cyclohexanecarboxylate (4s)
4-Chlorobenzyl cyclohexanecarboxylate (4t)
4-Methoxyphenyl cyclohexanecarboxylate (4u)
2-Bromophenyl butyrate (4w)

\[ \text{O} \quad \text{Br} \quad \text{O} \quad \text{Br} \]

\[ \text{O} \quad \text{O} \quad \text{Br} \]

X : parts per Million : Proton

X : parts per Million : Carbon13
$p$-Tolyl butyrate (4x)
Benzyl 3-methylbutanoate (4y)
4-Chlorophenyl 3-methylbutanoate (4z)

- Molecular structure of 4-Chlorophenyl 3-methylbutanoate (4z) is shown.
- The diagram includes the chemical structure with the chlorine atom (Cl) on the phenyl ring and the carboxylic acid functionality.
- The diagram also shows the proton (1H) and carbon (13C) NMR spectra with peaks labeled at specific ppm values.
- The proton NMR spectrum shows peaks at 7.342, 7.328, 7.260, 7.030, and 7.015 ppm.
- The carbon NMR spectrum shows peaks at 171.491, 149.296, 131.219, 129.582, and 123.119 ppm.
4-Methoxybenzyl 3-methylbutanoate (4aa)
Benzyl octanoate (4ab)
Heptyl pivalate (4ac)

![Graph of Heptyl pivalate (4ac)](image)

X : parts per Million : 1H

$\text{7.284}$  $\text{4.080}$  $\text{4.064}$  $\text{4.047}$  $\text{1.672}$  $\text{1.655}$  $\text{1.637}$  $\text{1.619}$  $\text{1.603}$  $\text{1.357}$  $\text{1.347}$  $\text{1.338}$  $\text{1.334}$  $\text{1.330}$  $\text{1.315}$  $\text{1.303}$  $\text{1.292}$  $\text{1.213}$  $\text{0.921}$  $\text{0.904}$  $\text{0.887}$

X : parts per Million : 13C

$\text{178.643}$  $\text{77.333}$  $\text{77.012}$  $\text{76.698}$  $\text{64.460}$  $\text{38.730}$  $\text{31.732}$  $\text{28.904}$  $\text{28.620}$  $\text{27.206}$  $\text{25.879}$  $\text{22.577}$  $\text{14.056}$
Thiophen-2-ylmethyl 3-methylbutanoate (4ad)
Butyl thiophene-2-carboxylate (4ae)
S-Cyclohexyl benzothioate (6a)

\[ \text{X : parts per Million : } { }^{1}H \]

\[ \begin{array}{cccccccccccccccccccc}
\end{array} \]

\[ \text{X : parts per Million : } { }^{13}C \]

\[ \begin{array}{cccccccccccccccccccc}
191.829 & 137.482 & 133.101 & 128.502 & 127.146 & 77.354 & 77.034 & 76.720 & 42.55 & 33.10 & 26.09 & 21.83 & 1.89 & 1.80 & 1.18 & 4.11
\end{array} \]
S-Phenyl benzothioate (6b)
S-Benzyl 4-methylbenzothioate (6c)

X : parts per Million : 1H

S

X : parts per Million : 13C

S

S

S

S

S

S
S-Benzyl 4-chlorobenzothioate (6d)
S-Butyl 4-chlorobenzothioate (6e)

![Diagram of S-Butyl 4-chlorobenzothioate (6e)]
S-Phenyl butanethioate (6f)
S-4-Chlorophenyl butanethioate (6g)
S-Benzyl 3-methylbutanethioate (6h)
S-p-Tolyl 3-methylbutanethioate (6i)