

# An expedient biocatalytic procedure for abasic site precursors useful in oligonucleotide synthesis

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<sup>‡</sup>Rasayan Inc., 2802 Crystal Ridge Road, Encinitas, CA 92024-6615, USA.

**ELECTRONIC SUPPLEMENTARY INFORMATION** (page 1 of 51 pages).

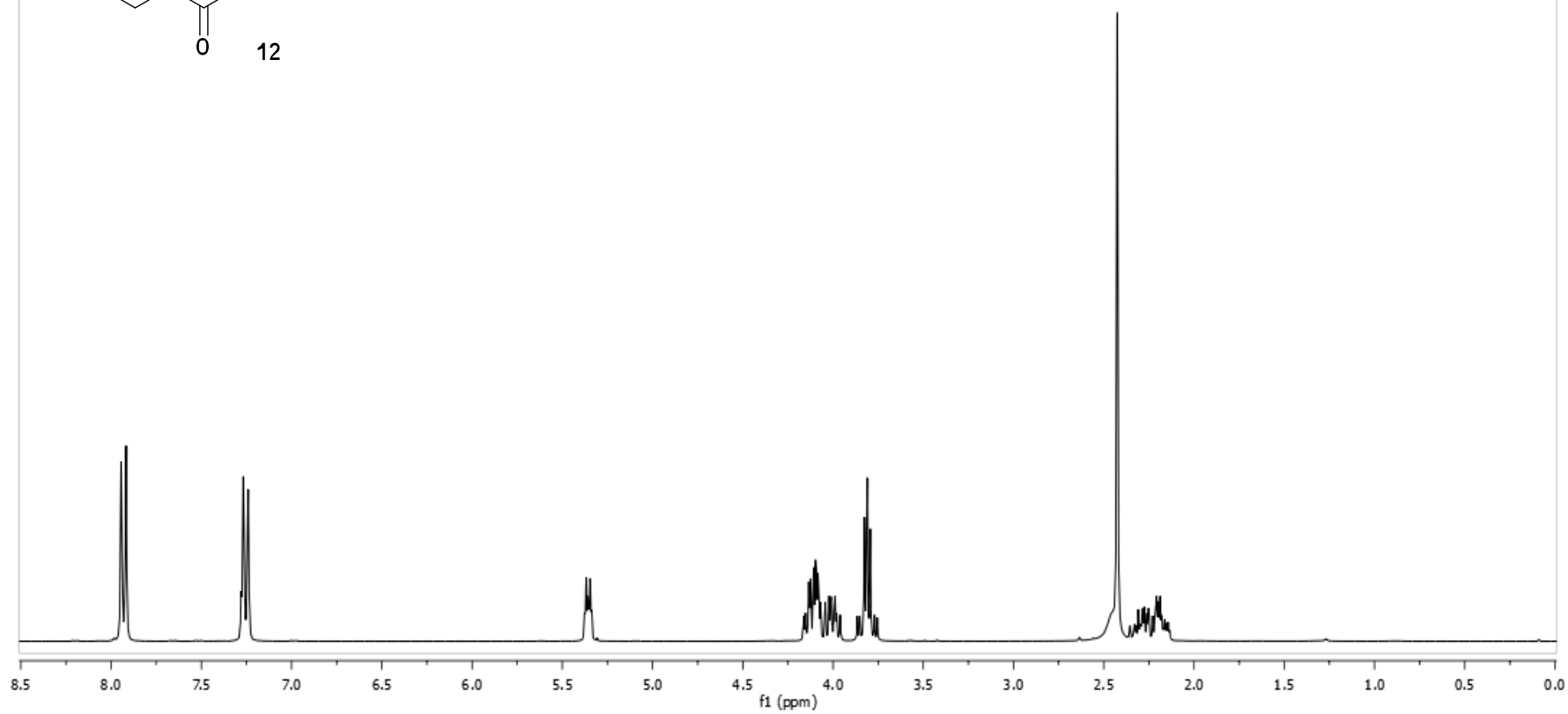
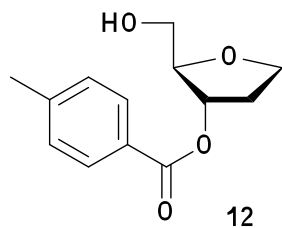
## Contents:

Copies of <sup>1</sup>H, <sup>13</sup>C, DEPT of compounds **12**, **13**, **14a-e**, **15a-e**, **16b-e**, **16**, **17**, **18a-b** and **19**.

- <sup>1</sup> H NMR of <b>12</b> (S2)	- DEPT NMR of <b>14e</b> (S19)	- <sup>19</sup> F NMR of <b>15e</b> (S36)
- <sup>13</sup> C NMR of <b>12</b> (S3)	- <sup>19</sup> F NMR of <b>14e</b> (S20)	- <sup>1</sup> H NMR of <b>16</b> (S37)
- DEPT NMR of <b>12</b> (S4)	- <sup>1</sup> H NMR of <b>15a</b> (S21)	- <sup>13</sup> C NMR of <b>16</b> (S38)
- <sup>1</sup> H NMR of <b>13</b> (S5)	- <sup>13</sup> C NMR of <b>15a</b> (S22)	- DEPT NMR of <b>16</b> (S39)
- <sup>13</sup> C NMR of <b>13</b> (S6)	- DEPT NMR of <b>15a</b> (S23)	- <sup>1</sup> H NMR of <b>17</b> (S40)
- DEPT NMR of <b>13</b> (S7)	- <sup>1</sup> H NMR of <b>15b</b> (S24)	- <sup>13</sup> C NMR of <b>17</b> (S41)
- <sup>1</sup> H NMR of <b>14b</b> (S8)	- <sup>13</sup> C NMR of <b>15b</b> (S25)	- DEPT NMR of <b>17</b> (S42)
- <sup>13</sup> C NMR of <b>14b</b> (S9)	- DEPT NMR of <b>15b</b> (S26)	- <sup>1</sup> H NMR of <b>18a</b> (S43)
- DEPT NMR of <b>14b</b> (S10)	- <sup>1</sup> H NMR of <b>15c</b> (S27)	- <sup>13</sup> C NMR of <b>18a</b> (S44)
- <sup>1</sup> H NMR of <b>14c</b> (S11)	- <sup>13</sup> C NMR of <b>15c</b> (S28)	- DEPT NMR of <b>18a</b> (S45)
- <sup>13</sup> C NMR of <b>14c</b> (S12)	- DEPT NMR of <b>15c</b> (S29)	- <sup>1</sup> H NMR of <b>18b</b> (S46)
- DEPT NMR of <b>14c</b> (S13)	- <sup>1</sup> H NMR of <b>15d</b> (S30)	- <sup>13</sup> C NMR of <b>18b</b> (S47)
- <sup>1</sup> H NMR of <b>14d</b> (S14)	- <sup>13</sup> C NMR of <b>15d</b> (S31)	- DEPT NMR of <b>19</b> (S48)
- <sup>13</sup> C NMR of <b>14d</b> (S15)	- DEPT NMR of <b>15d</b> (S32)	- <sup>1</sup> H NMR of <b>19</b> (S49)
- DEPT NMR of <b>14d</b> (S16)	- <sup>1</sup> H NMR of <b>15e</b> (S33)	- <sup>13</sup> C NMR of <b>19</b> (S50)
- <sup>1</sup> H NMR of <b>14e</b> (S17)	- <sup>13</sup> C NMR of <b>15e</b> (S34)	- DEPT NMR of <b>19</b> (S51)
- <sup>13</sup> C NMR of <b>14e</b> (S18)	- DEPT NMR of <b>15e</b> (S35)	

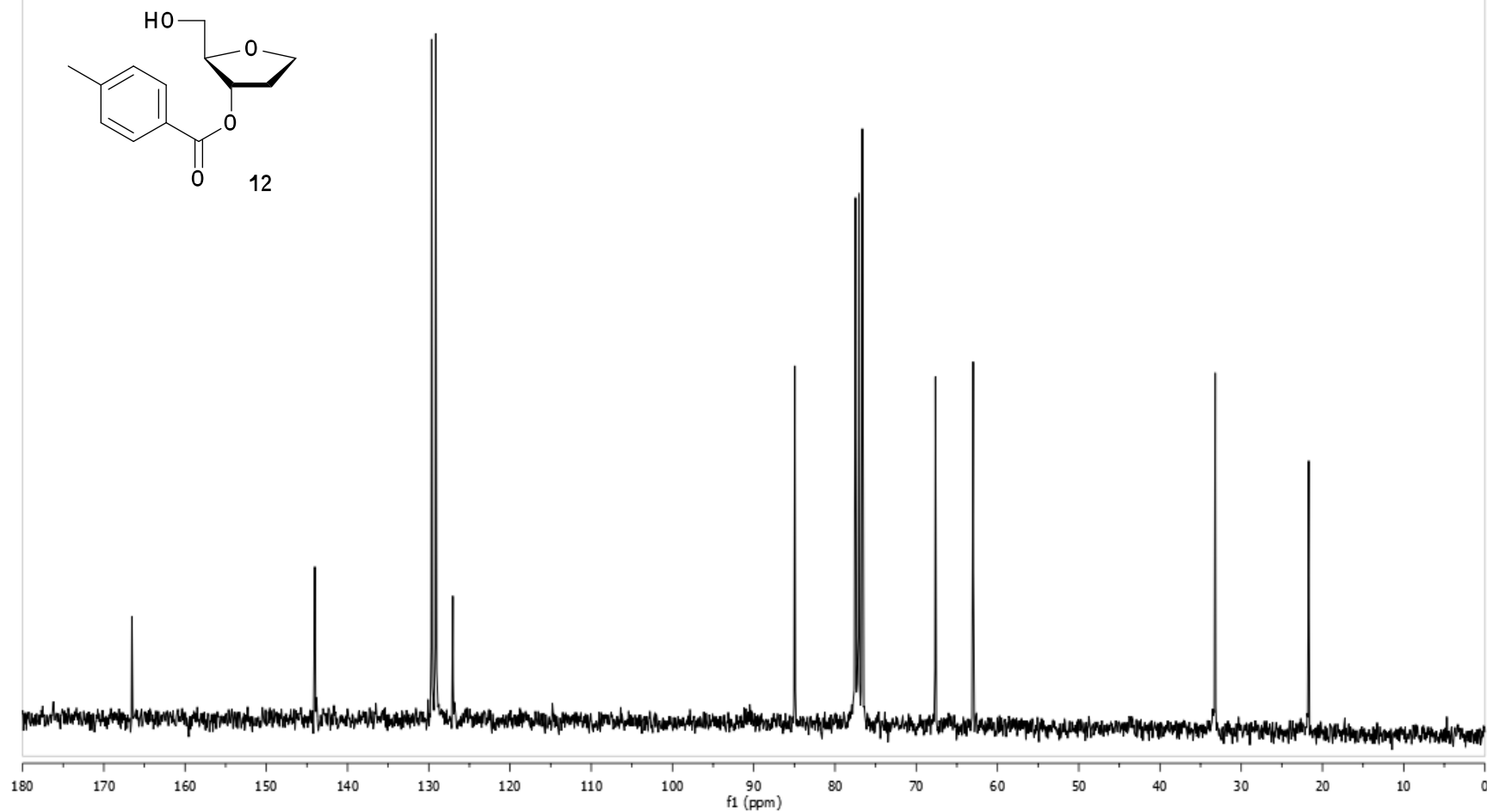
### 3-O-Toluoyl-1,2-dideoxy-D-ribose (12)

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300.13 MHz)



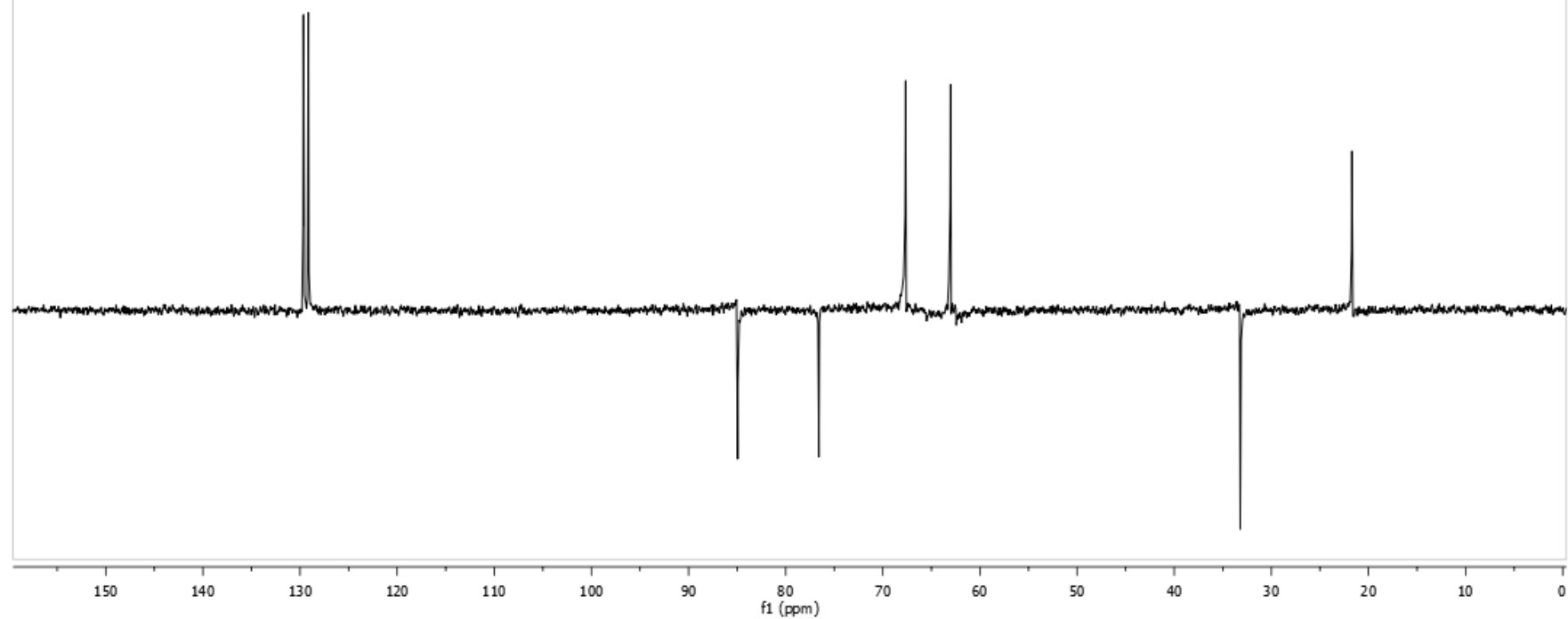
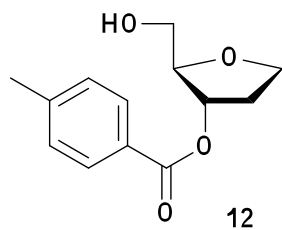
# 3-O-Toluoyl-1,2-dideoxy-D-ribose (12)

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75.5 MHz)



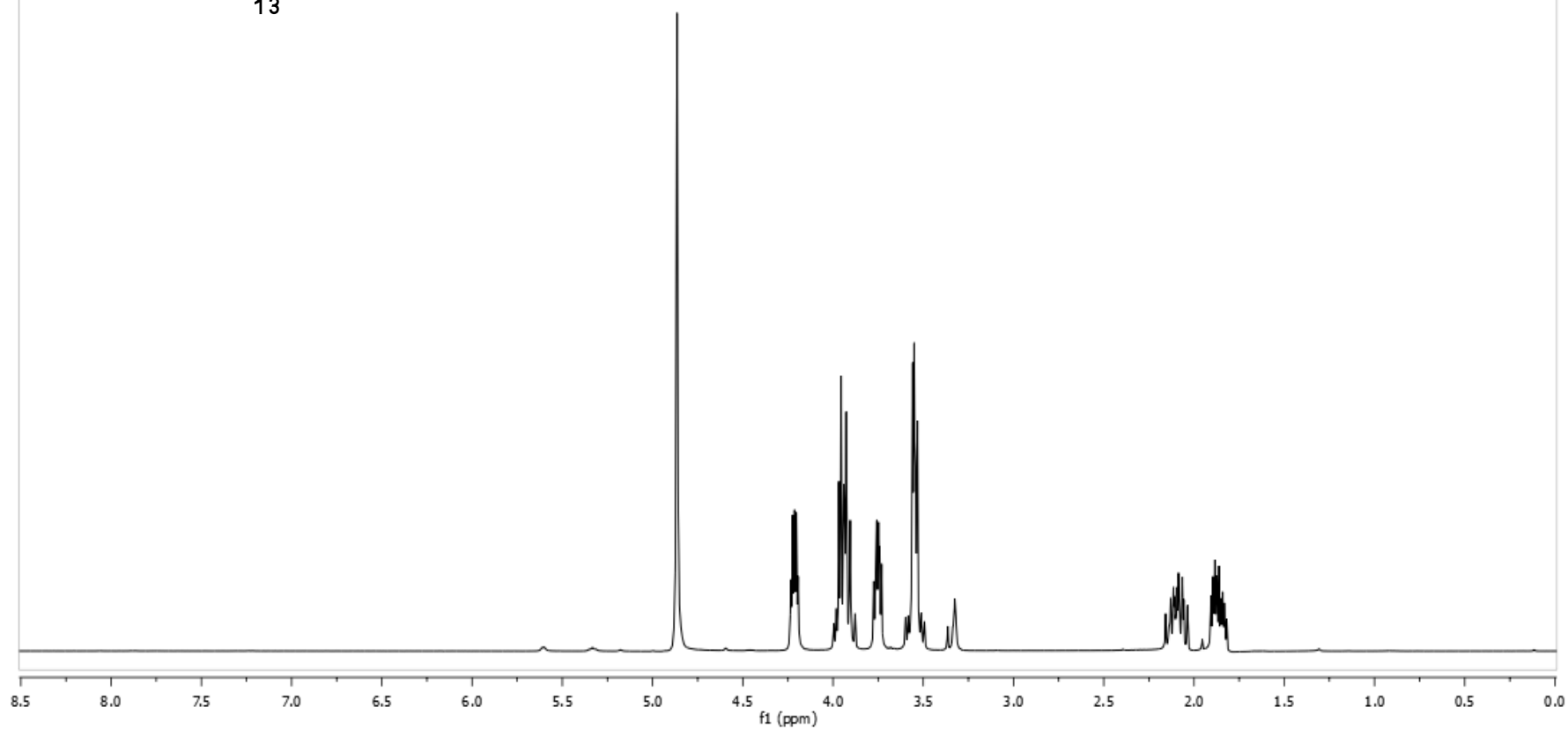
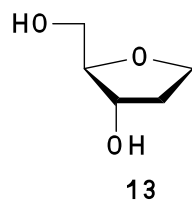
### 3-O-Toluoyl-1,2-dideoxy-D-ribose (12)

DEPT NMR ( $\text{CDCl}_3$ , 75.5 MHz)



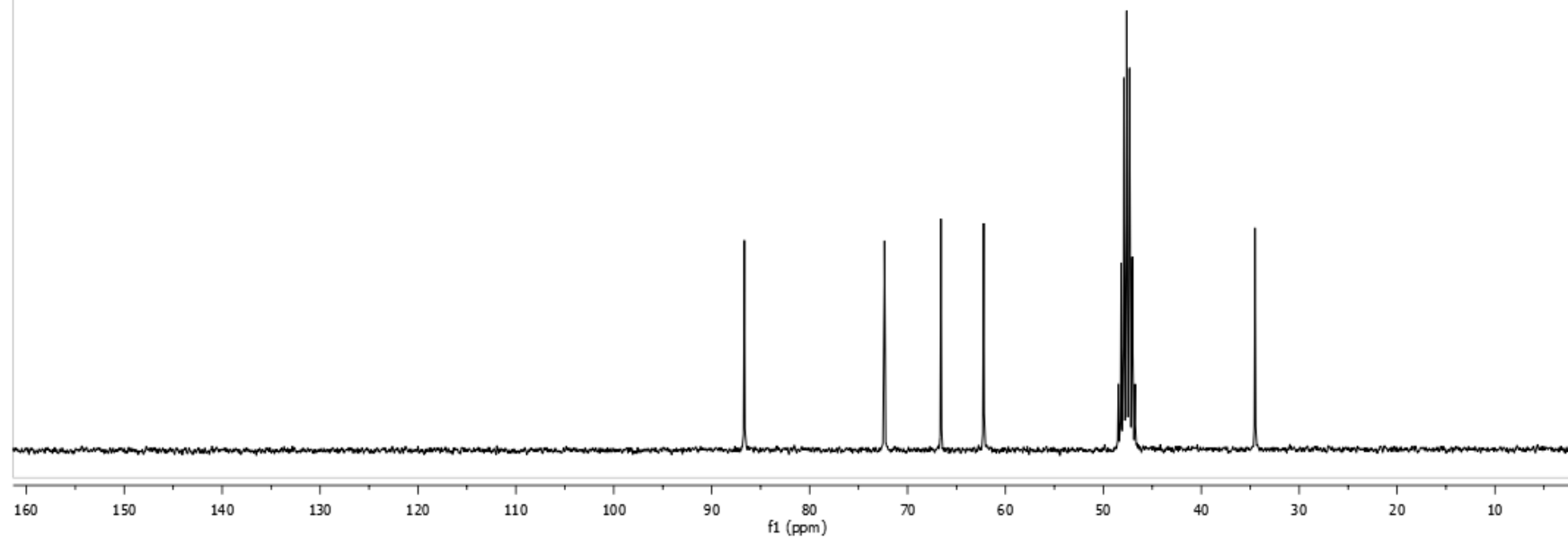
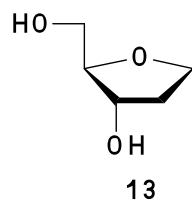
## 1,2-Dideoxy-D-ribose (13)

$^1\text{H}$  NMR (MeOH- $d_4$ , 300.13 MHz)



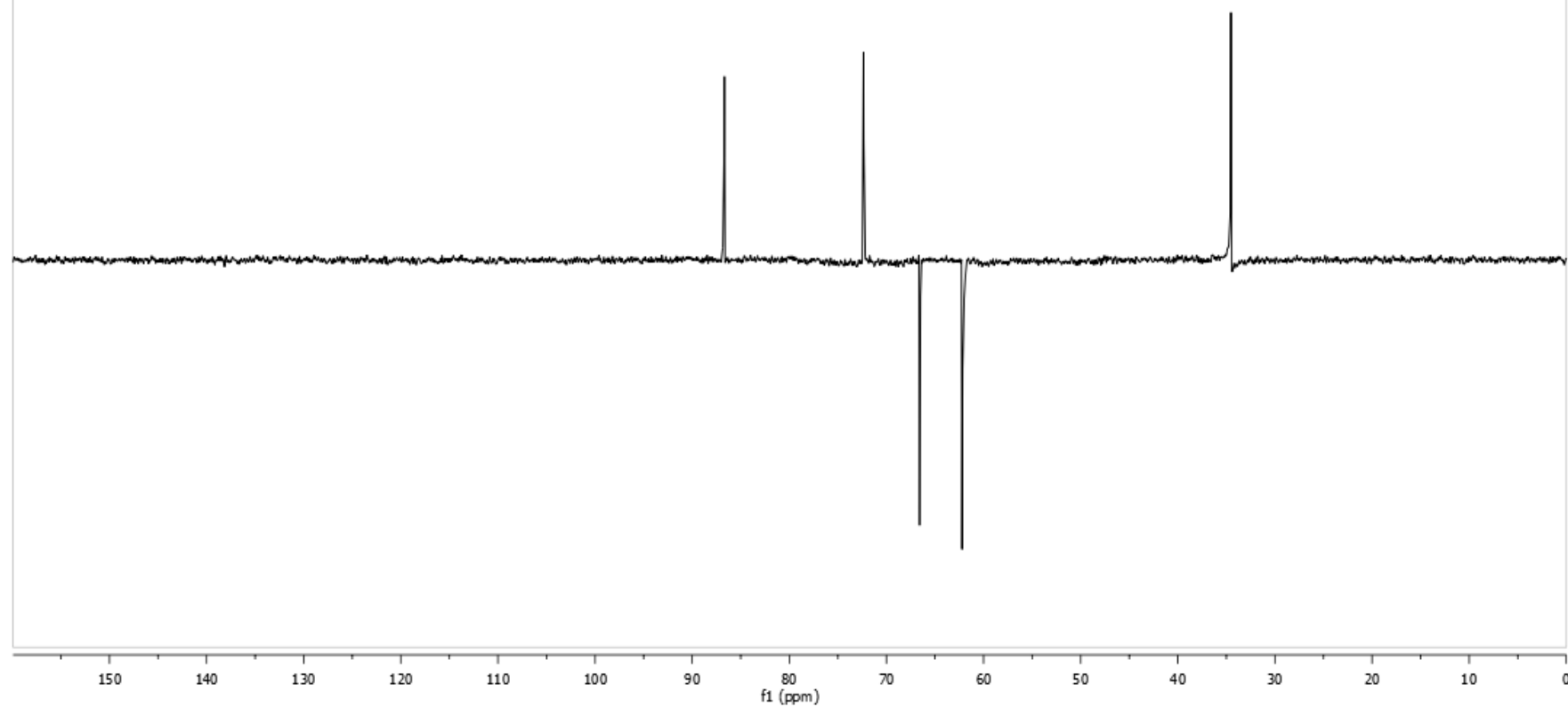
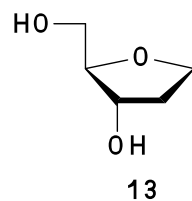
## 1,2-Dideoxy-D-ribose (13)

$^{13}\text{C}$  NMR (MeOH- $d_4$ , 75.5 MHz)



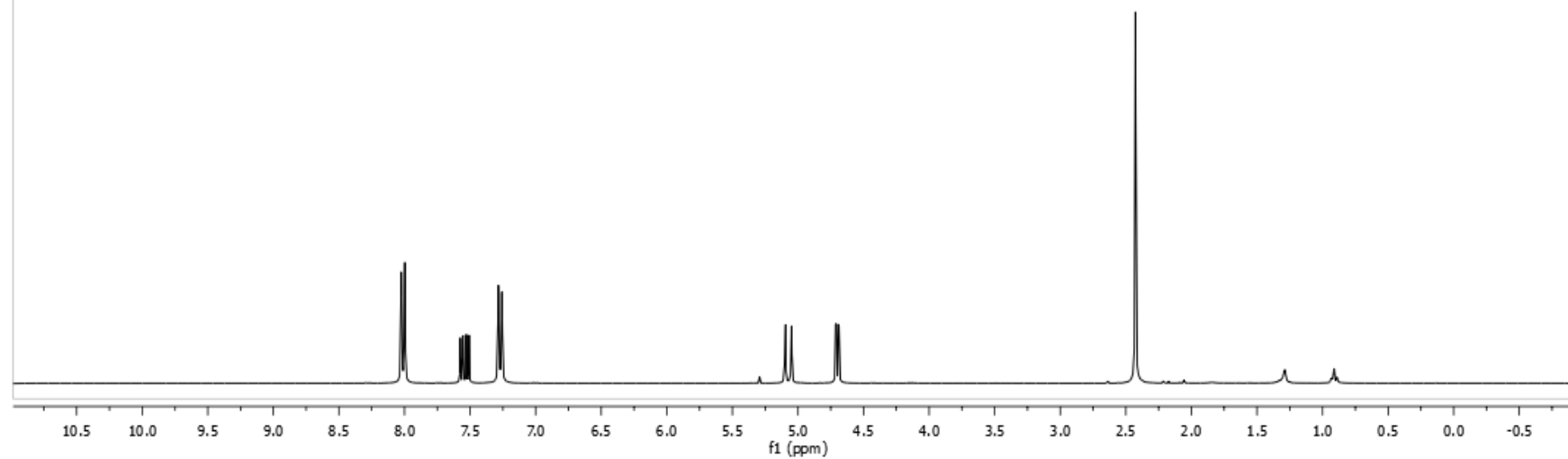
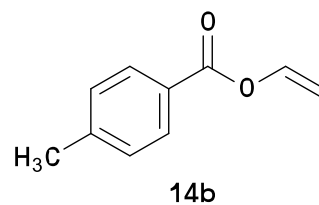
## 1,2-Dideoxy-D-ribose (13)

DEPT NMR (MeOH- $d_4$ , 75.5 MHz)



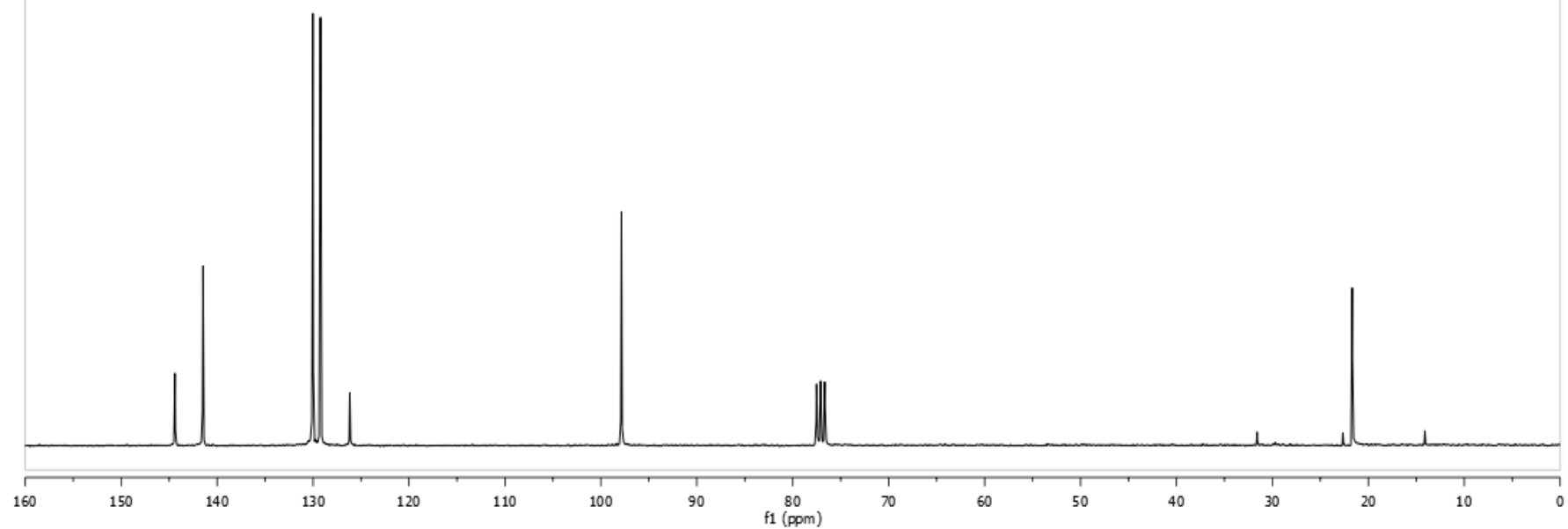
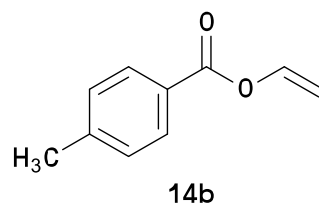
## Vinyl 4-methylbenzoate (14b)

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300.13 MHz)



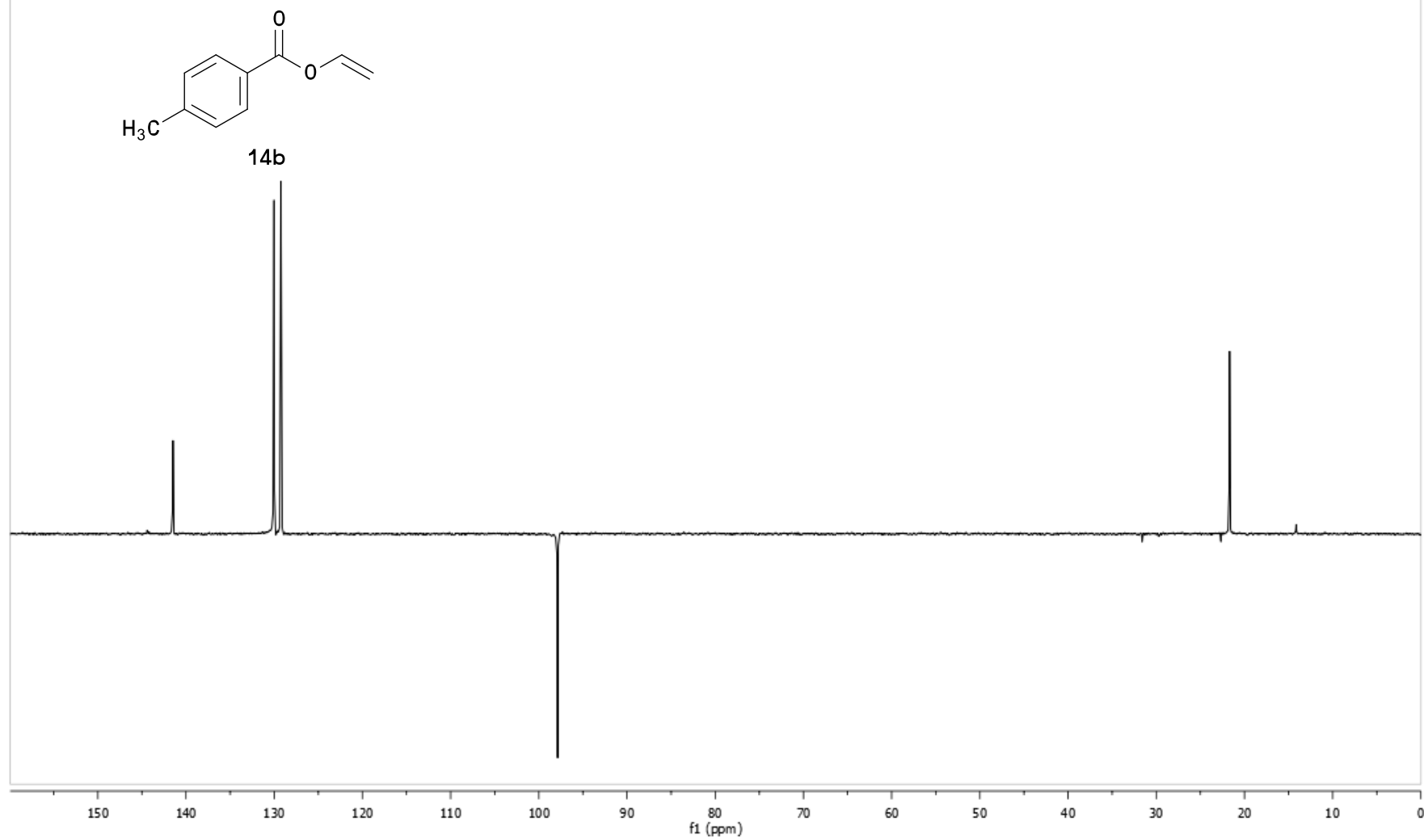
## Vinyl 4-methylbenzoate (14b)

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75.5 MHz)



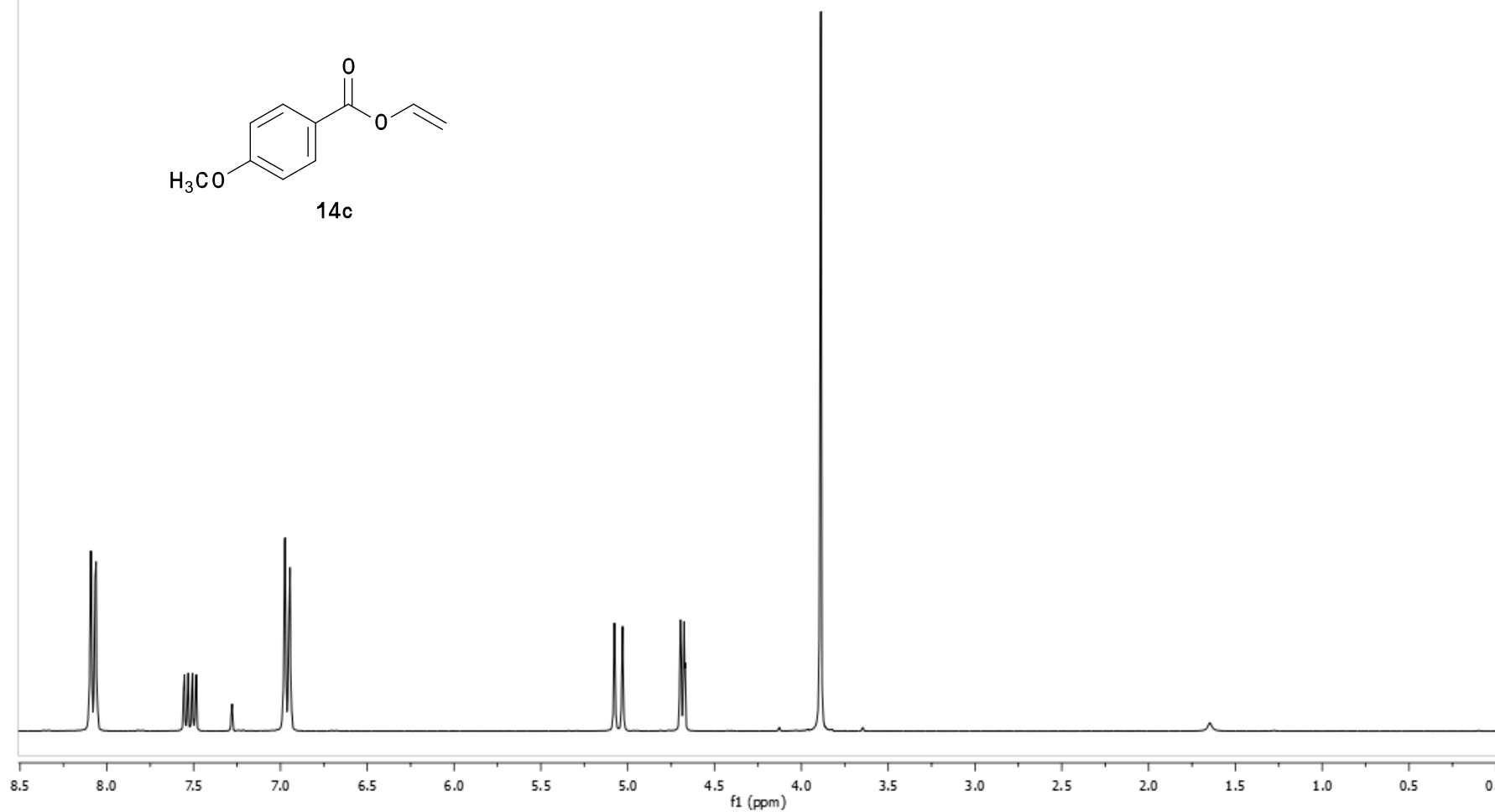
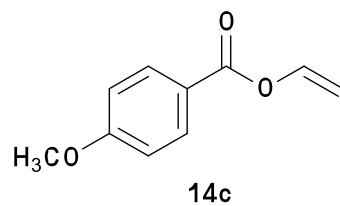
## Vinyl 4-methylbenzoate (14b)

DEPT NMR ( $\text{CDCl}_3$ , 75.5 MHz)



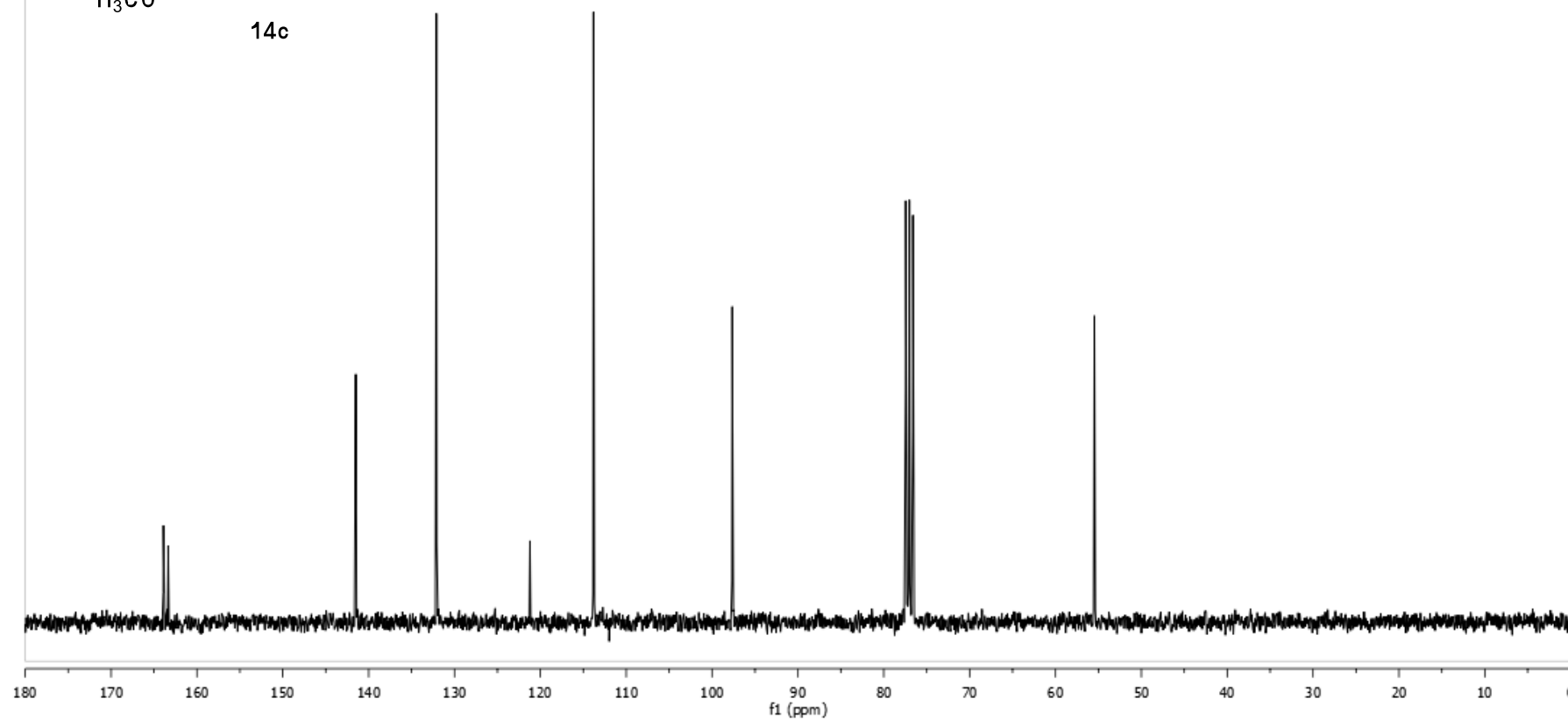
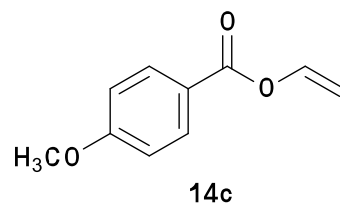
## Vinyl 4-methoxybenzoate (14c)

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300.13 MHz)



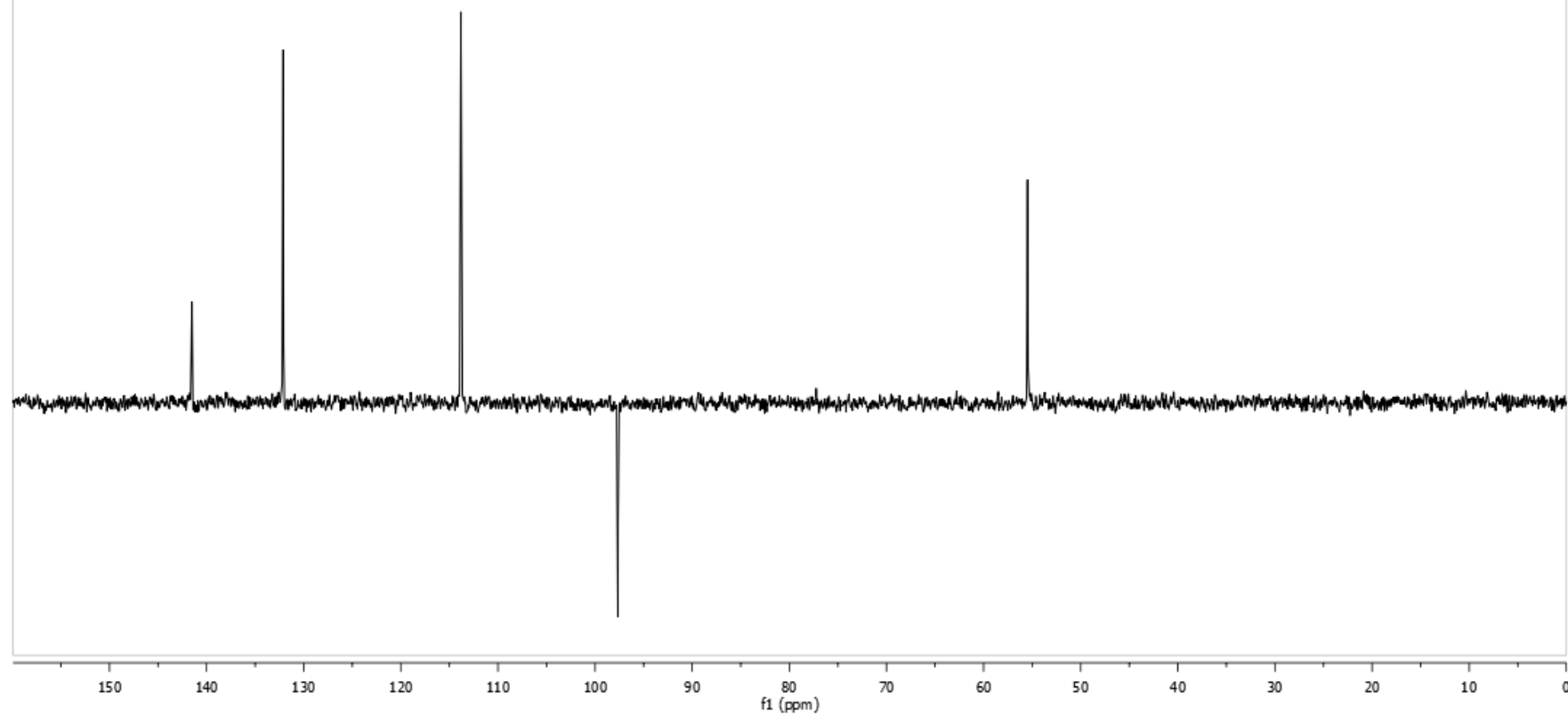
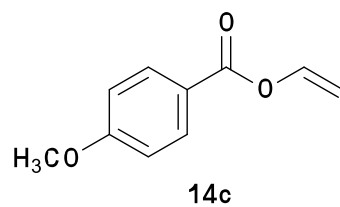
## Vinyl 4-methoxybenzoate (14c)

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75.5 MHz)



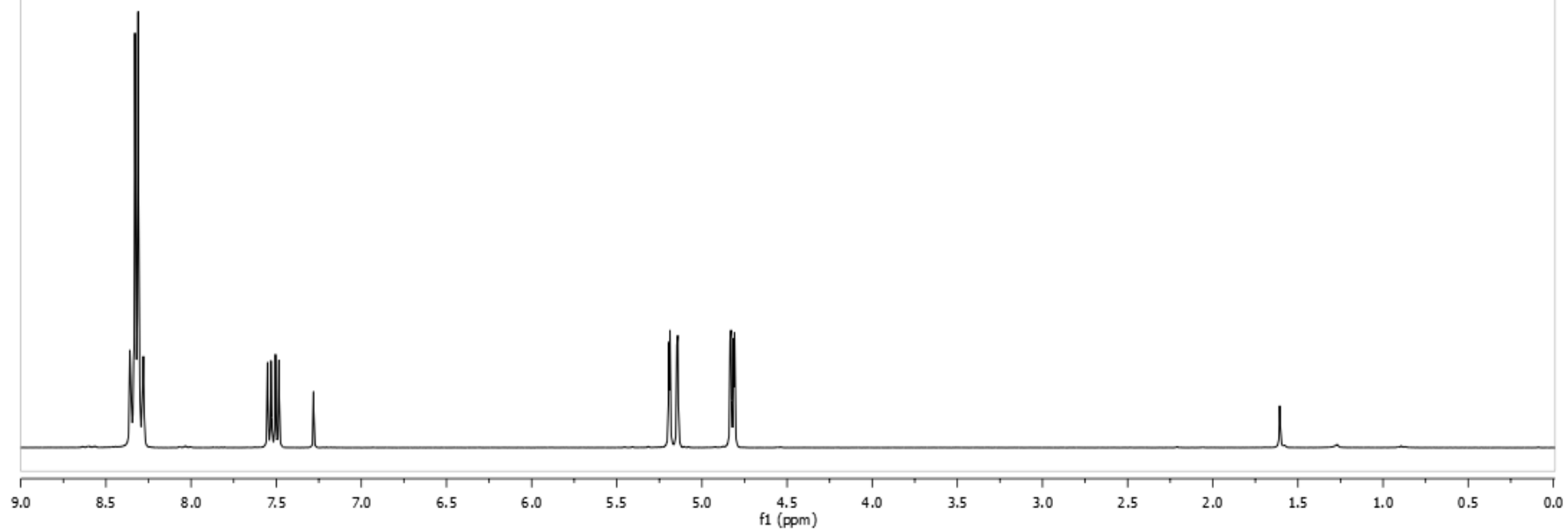
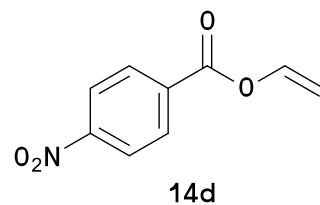
## Vinyl 4-methoxybenzoate (14c)

DEPT NMR ( $\text{CDCl}_3$ , 75.5 MHz)



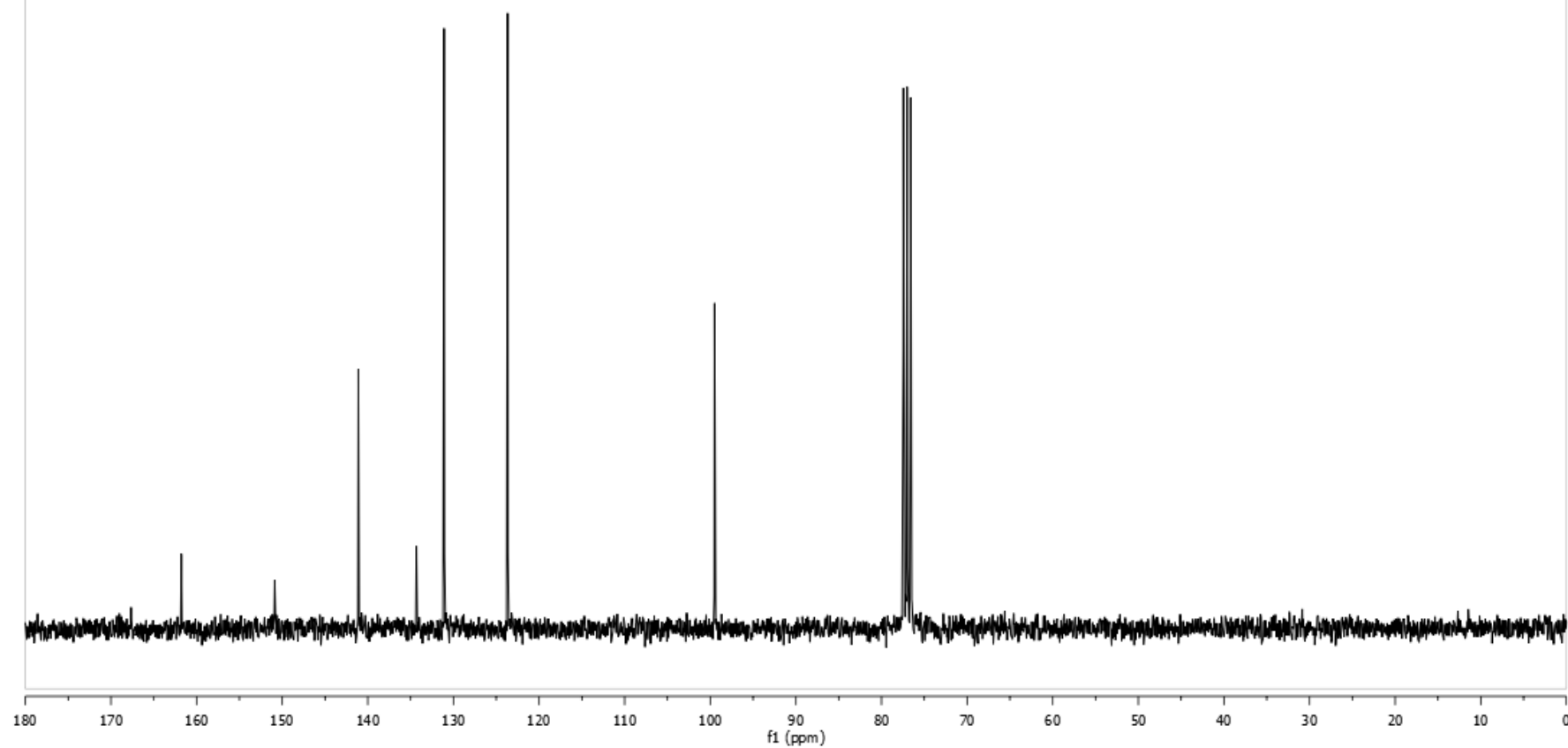
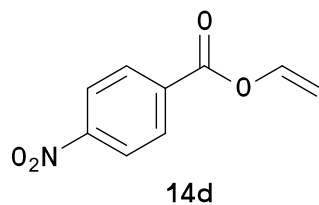
## Vinyl 4-nitrobenzoate (14d)

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300.13 MHz)



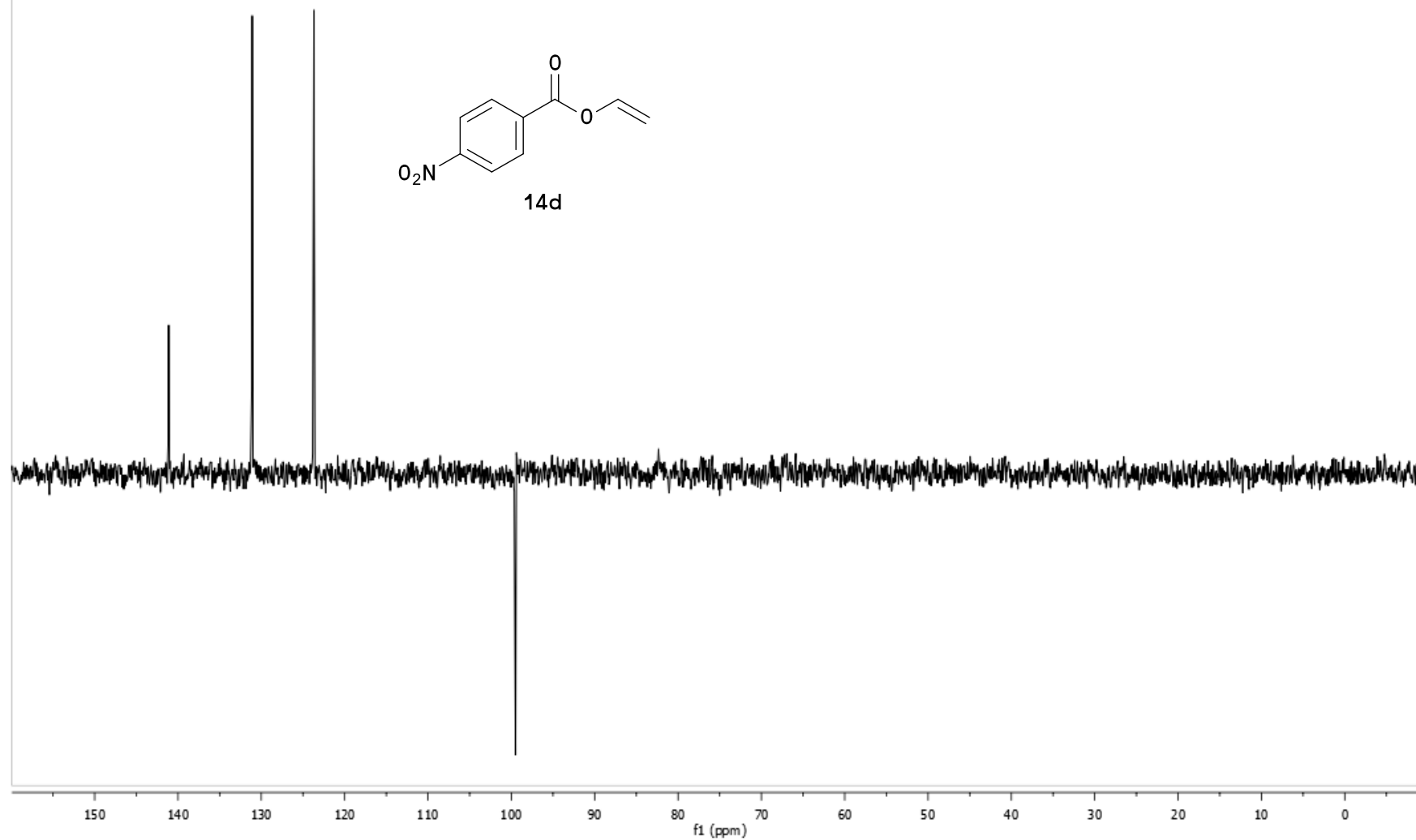
## Vinyl 4-nitrobenzoate (14d)

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75.5 MHz)



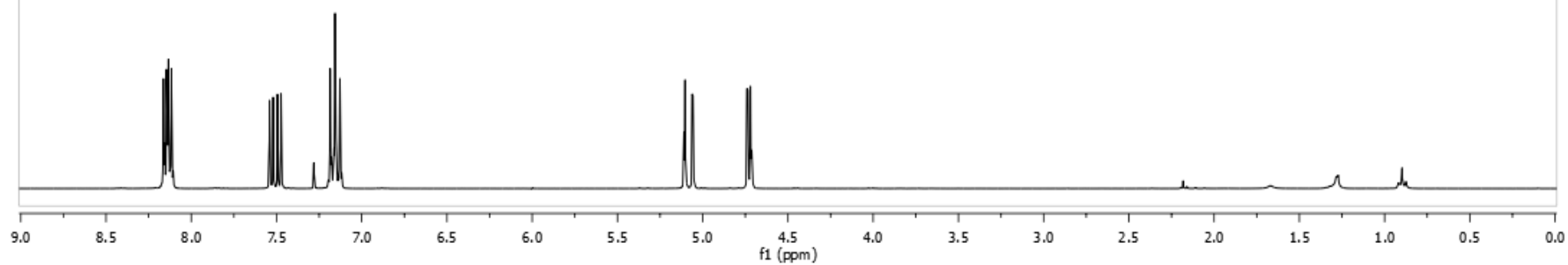
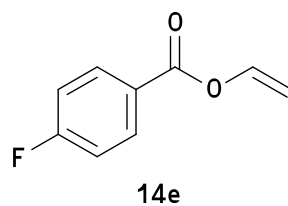
## Vinyl 4-nitrobenzoate (14d)

DEPT NMR ( $\text{CDCl}_3$ , 75.5 MHz)



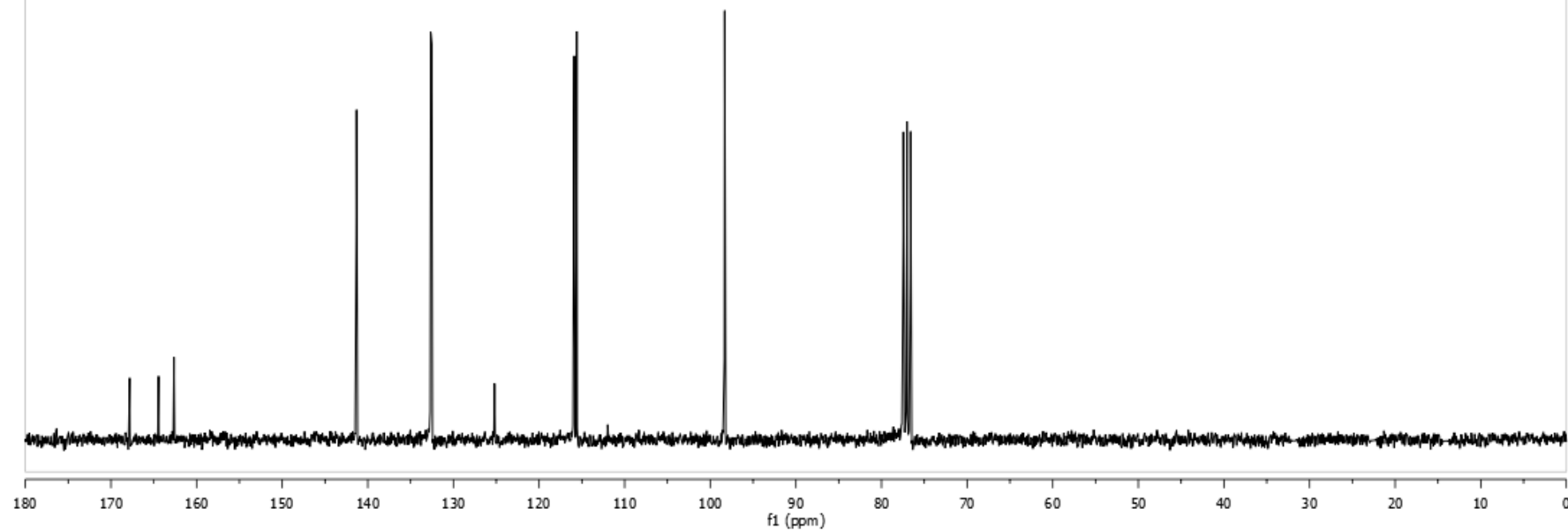
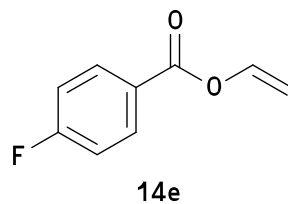
## Vinyl 4-fluorobenzoate (14d)

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300.13 MHz)



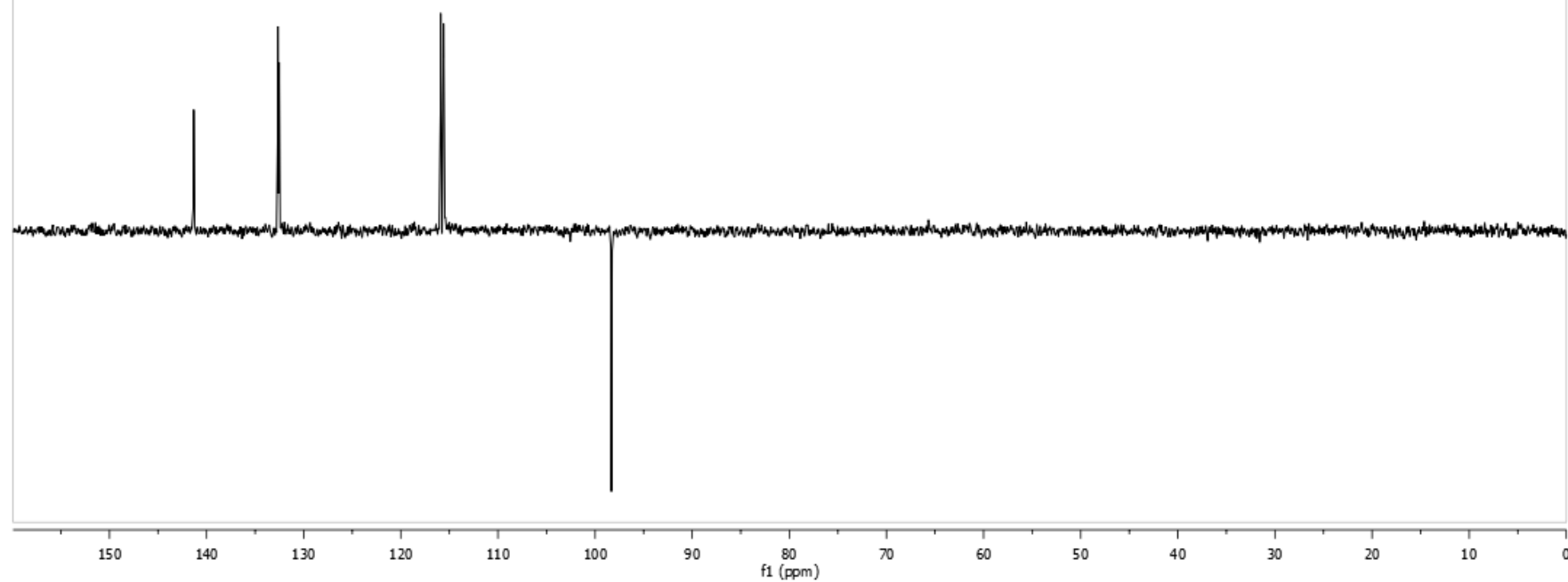
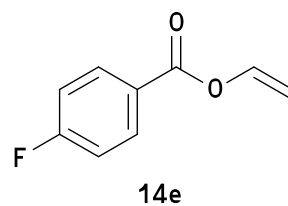
## Vinyl 4-fluorobenzoate (14e)

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75.5 MHz)



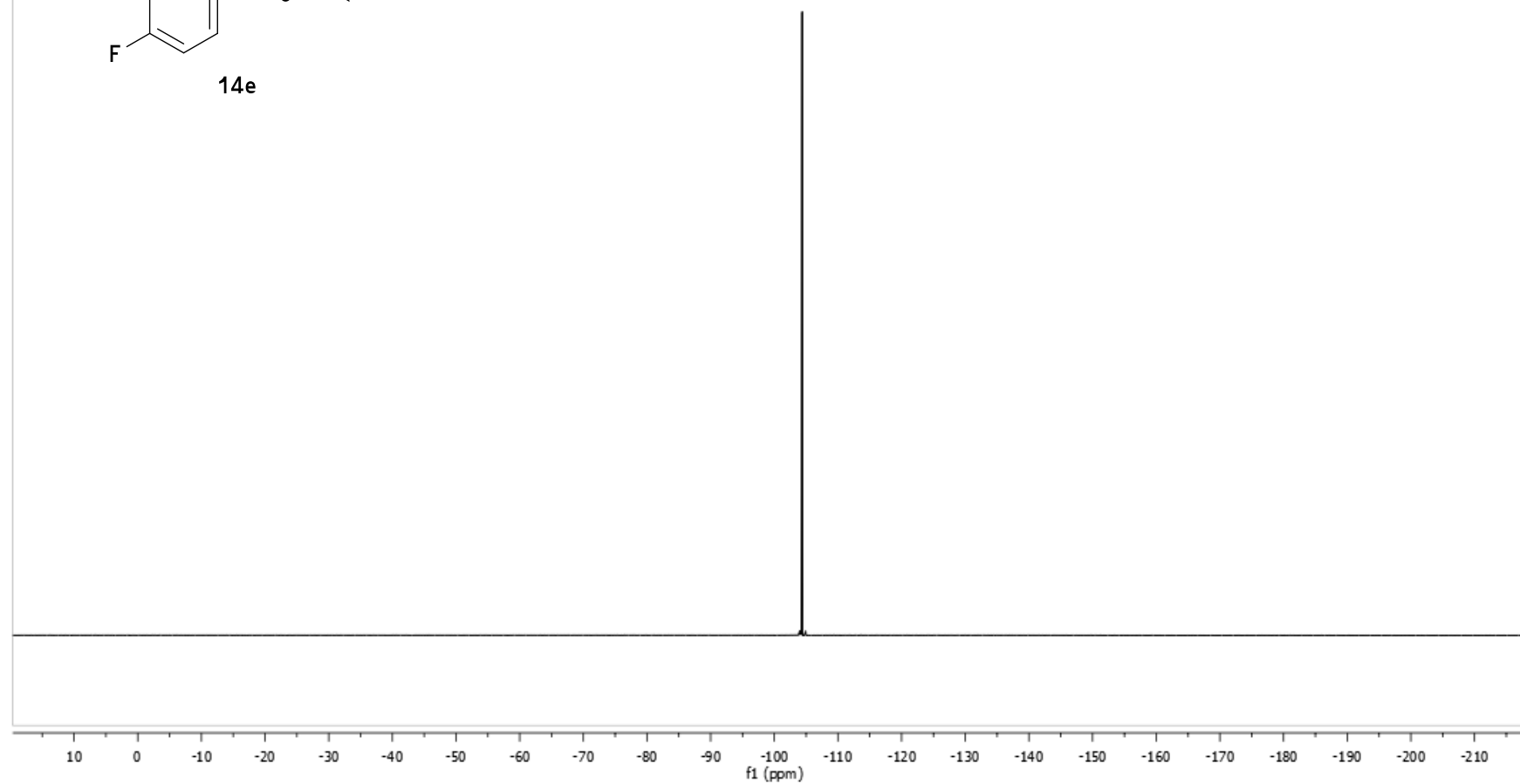
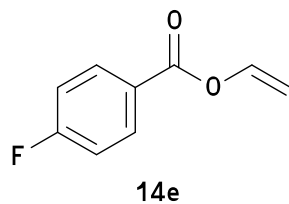
## Vinyl 4-fluorobenzoate (14e)

DEPT NMR ( $\text{CDCl}_3$ , 75.5 MHz)



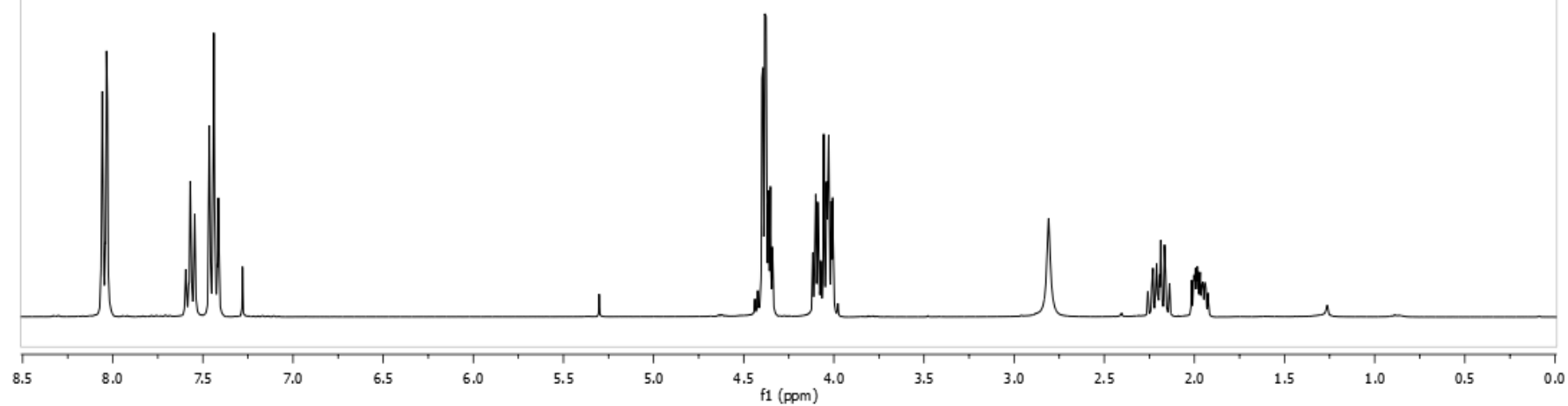
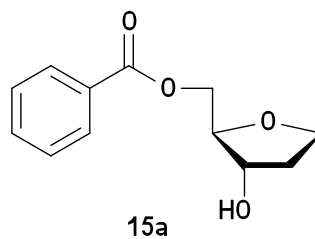
## Vinyl 4-fluorobenzoate (14e)

$^{19}\text{F}$  NMR ( $\text{CDCl}_3$ , 282.38 MHz)



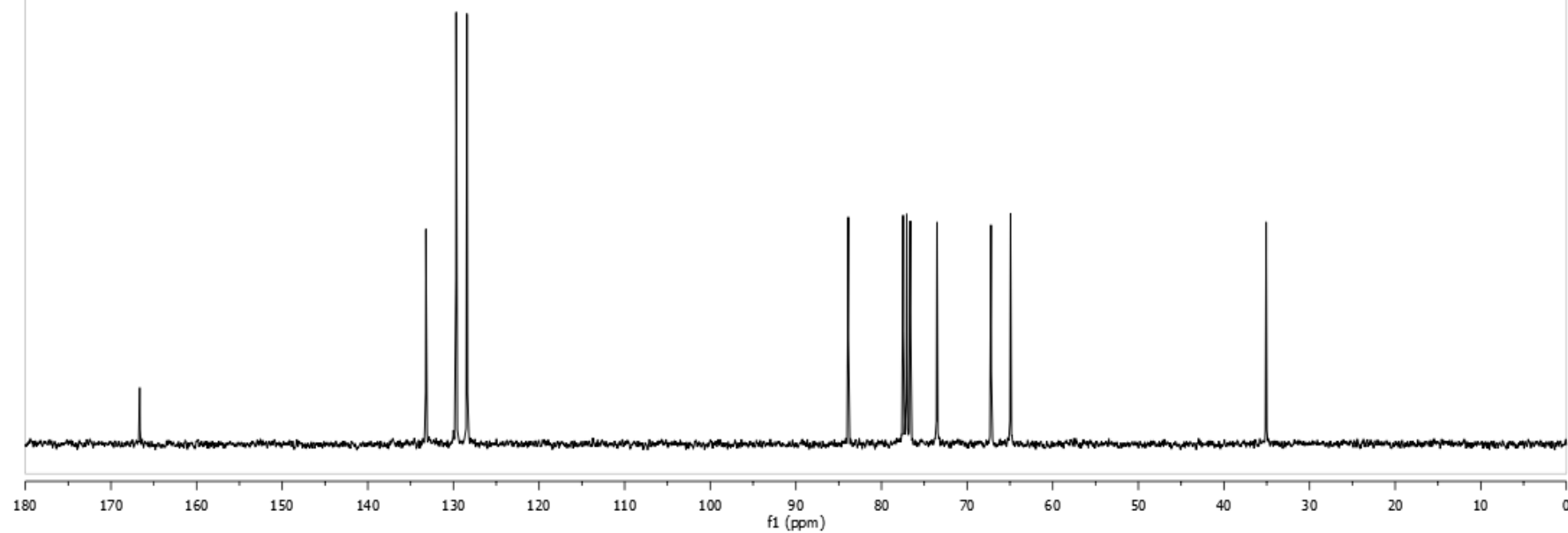
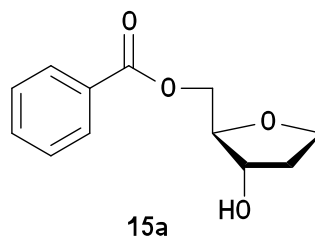
## 5-O-Benzoyl-1,2-dideoxy-D-ribose (15a)

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300.13 MHz)



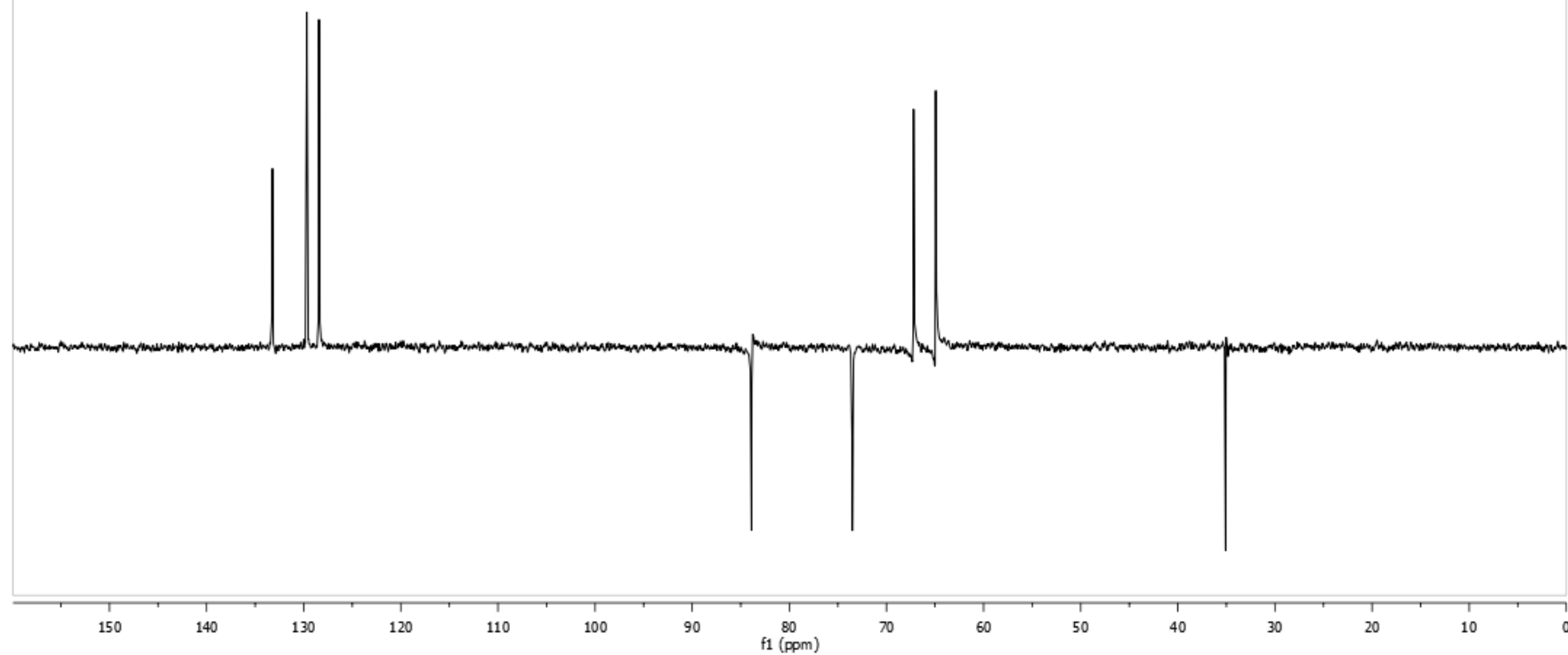
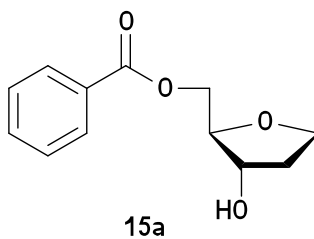
## 5-O-Benzoyl-1,2-dideoxy-D-ribose (15a)

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75.5 MHz)



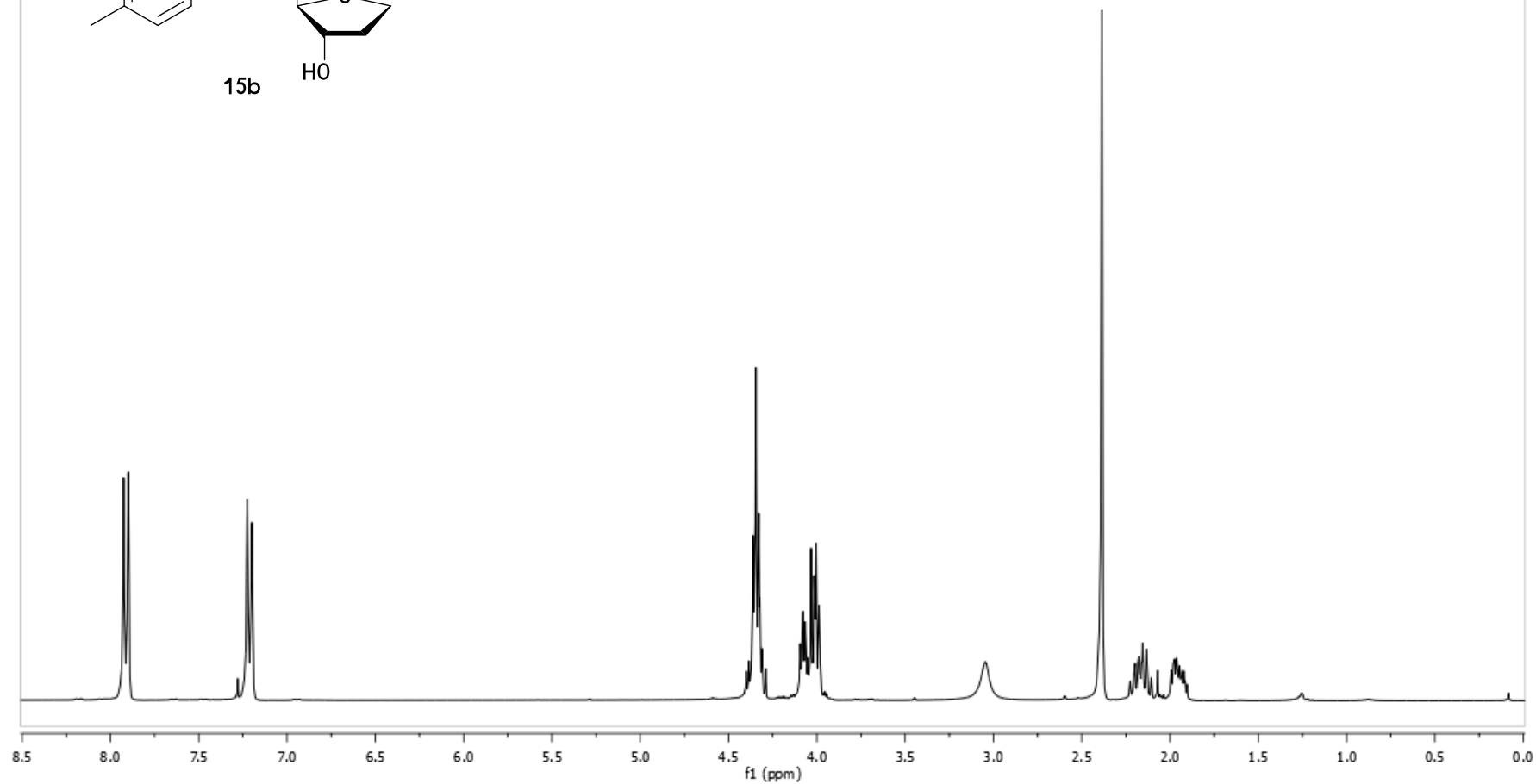
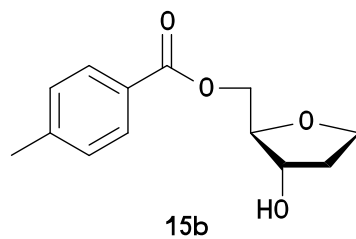
## 5-O-Benzoyl-1,2-dideoxy-D-ribose (15a)

DEPT NMR ( $\text{CDCl}_3$ , 75.5 MHz)



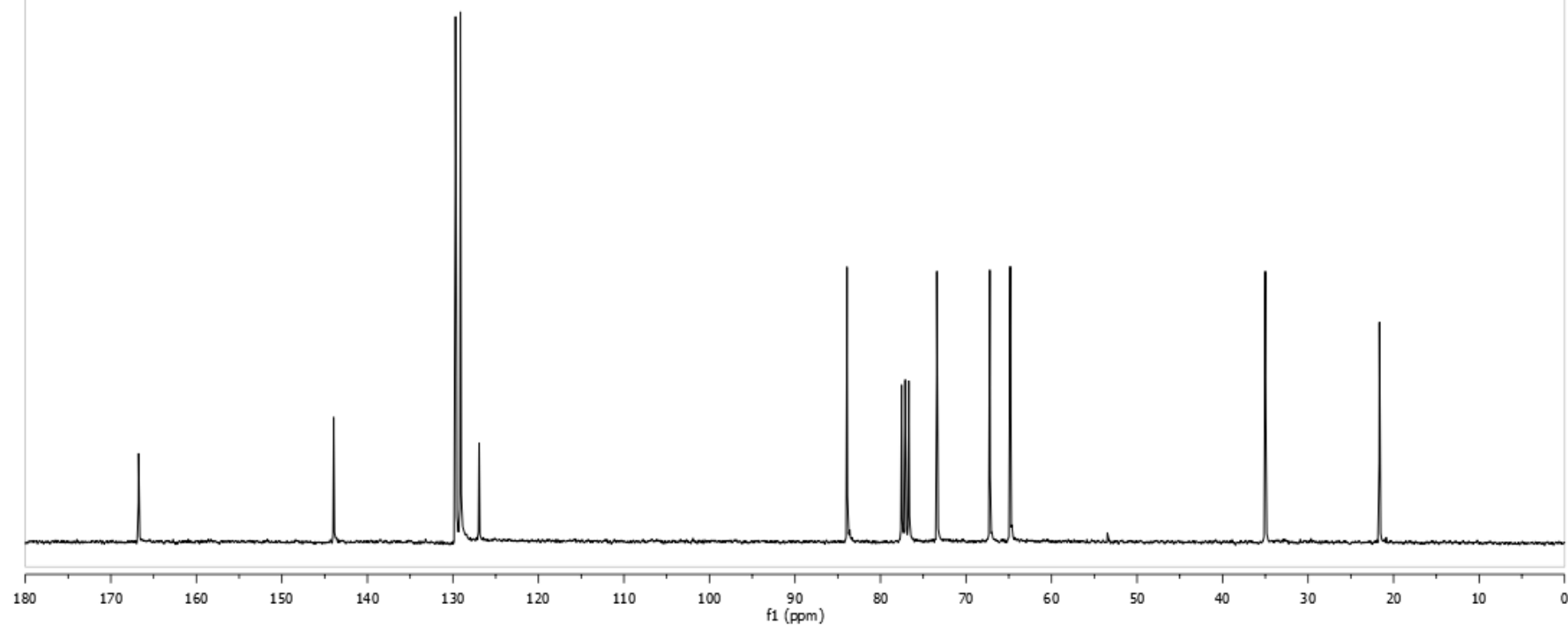
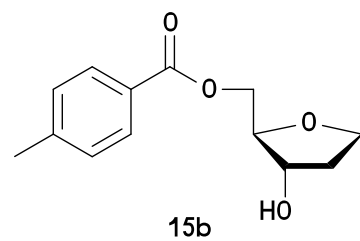
## 5-O-Toluoyl-1,2-dideoxy-D-ribose (15b)

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300.13 MHz)



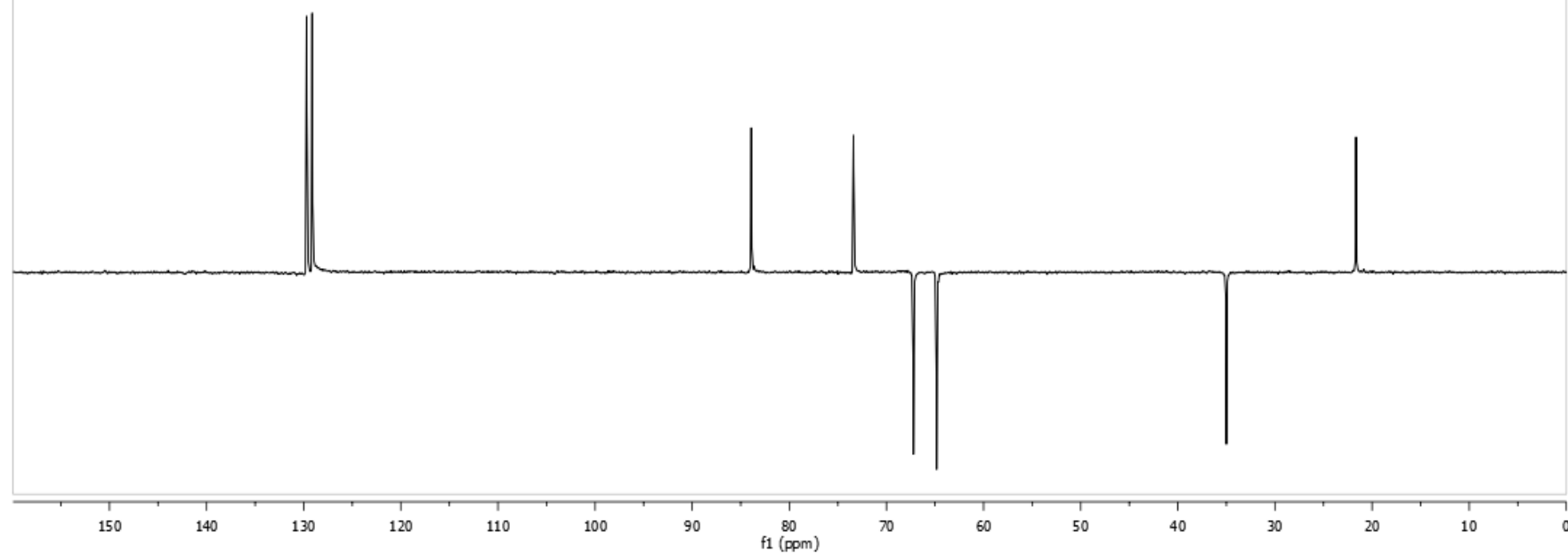
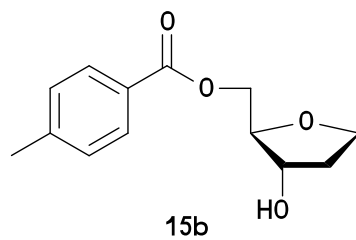
## 5-O-Toluoyl-1,2-dideoxy-D-ribose (15b)

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75.5 MHz)



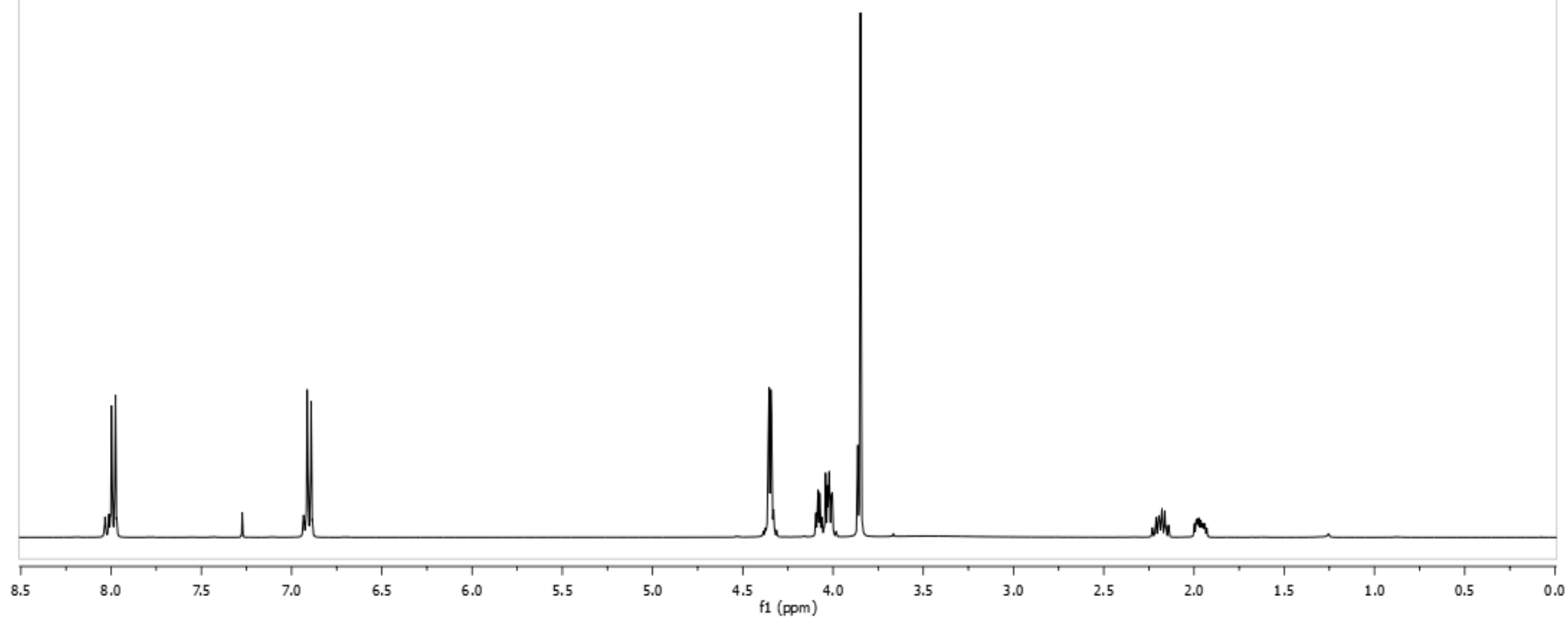
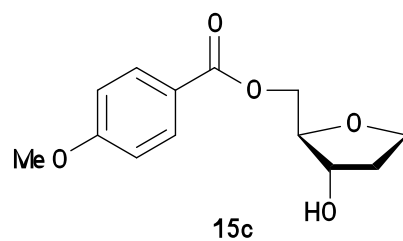
## 5-O-Toluoyl-1,2-dideoxy-D-ribose (15b)

DEPT NMR ( $\text{CDCl}_3$ , 75.5 MHz)



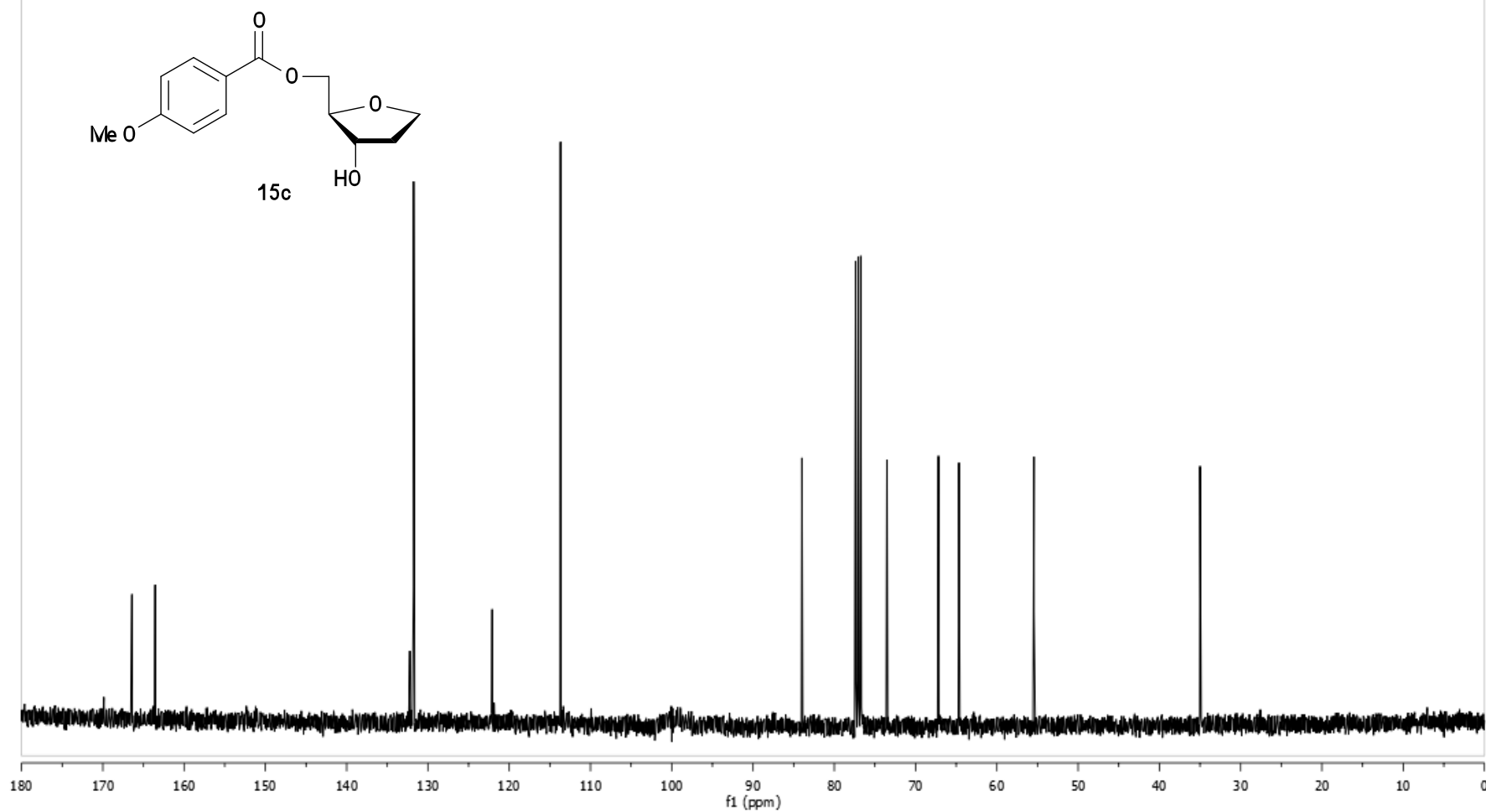
## 5-*O*-*p*-Methoxybenzoyl-1,2-dideoxy-D-ribose (15c)

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400.13 MHz)



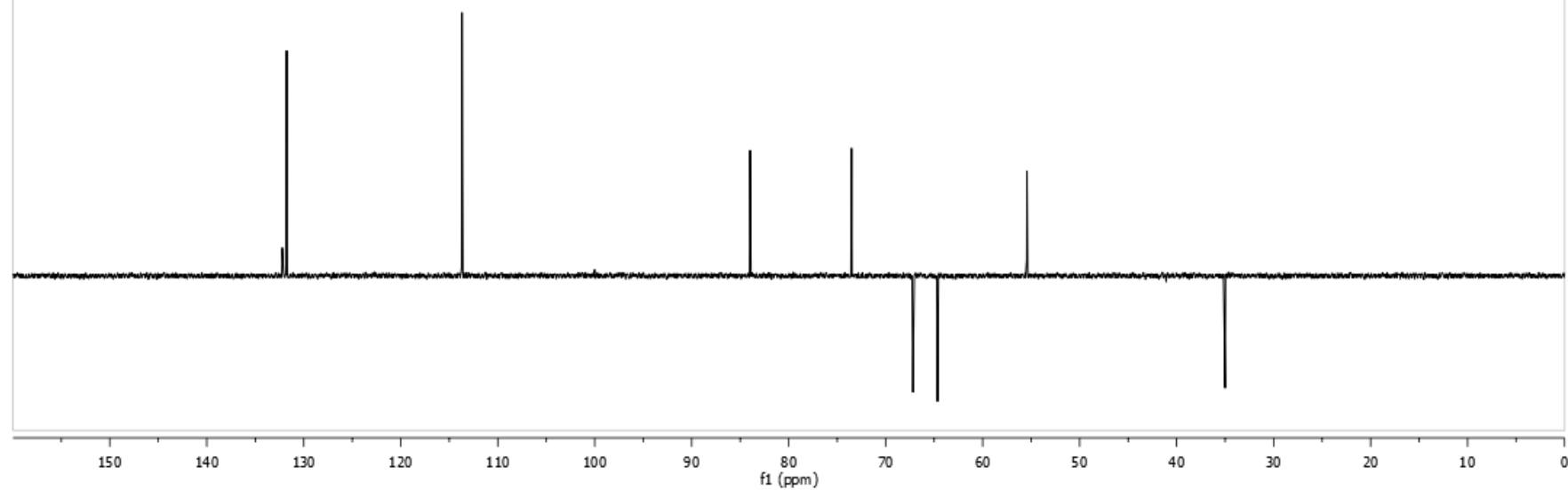
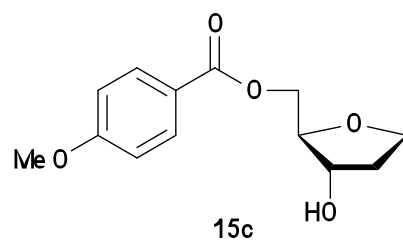
## 5-*O*-*p*-Methoxybenzoyl-1,2-dideoxy-D-ribose (15c)

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100.61 MHz)



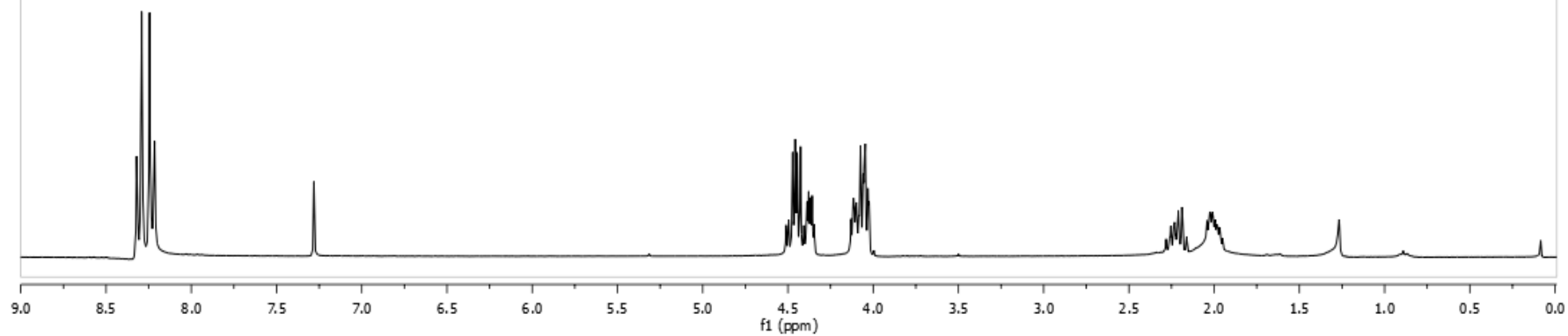
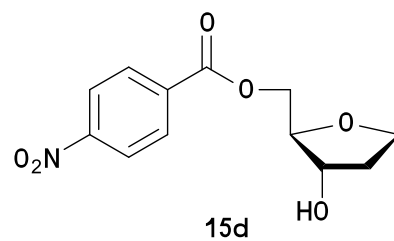
## 5-*O*-*p*-Methoxybenzoyl-1,2-dideoxy-D-ribose (15c)

$^{13}\text{C}$ DEPT NMR ( $\text{CDCl}_3$ , 100.61 MHz)



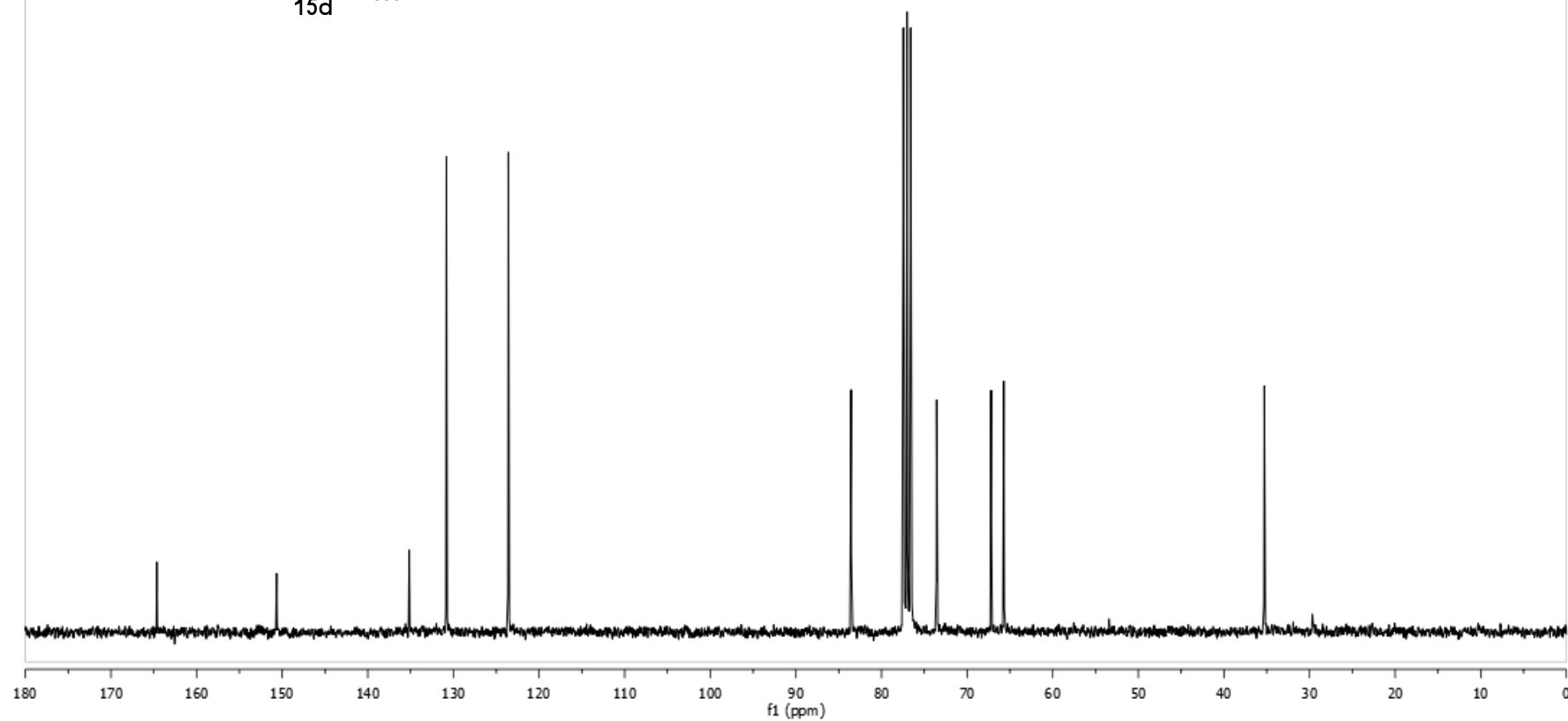
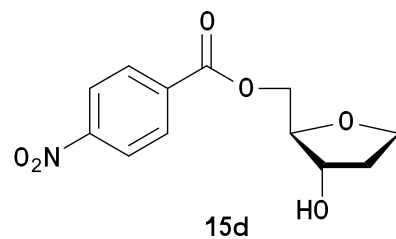
## 5-*O*-*p*-Nitrobenzoyl-1,2-dideoxy-D-ribose (15d)

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300.13 MHz)



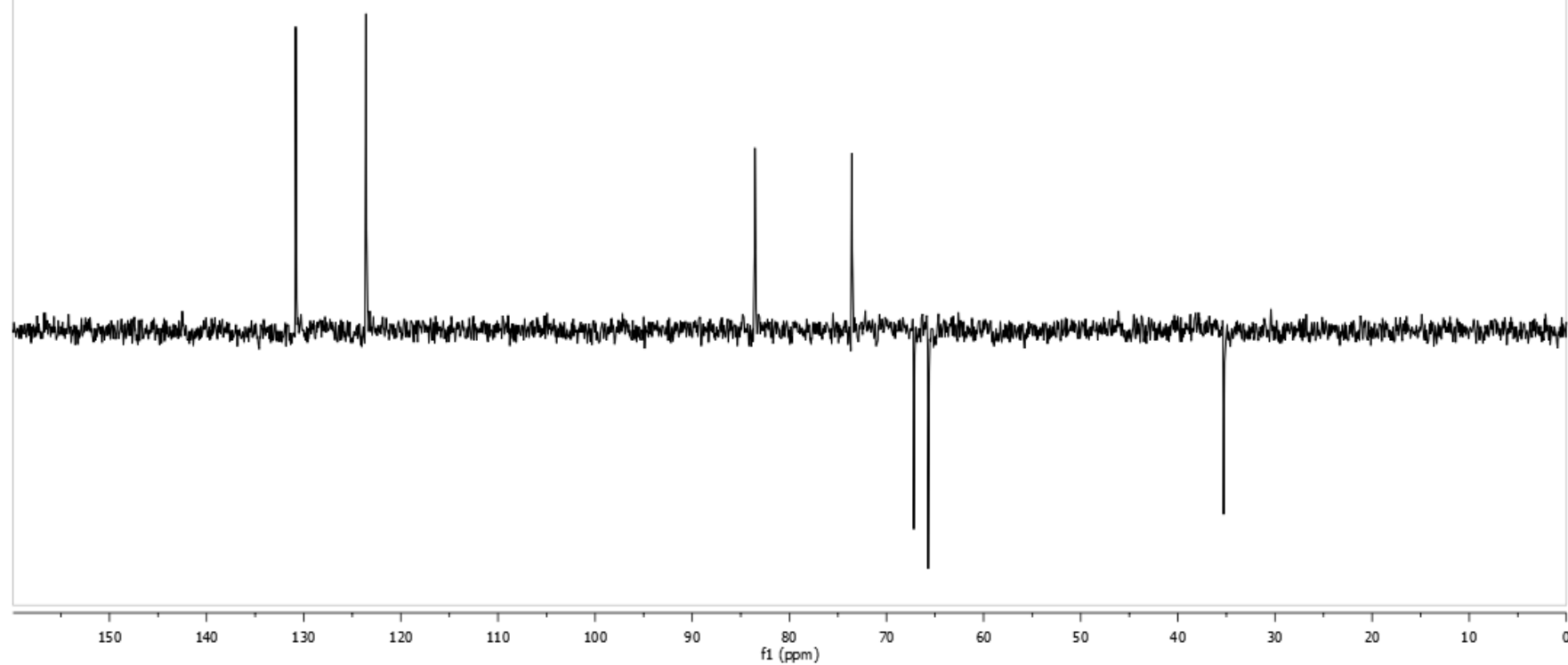
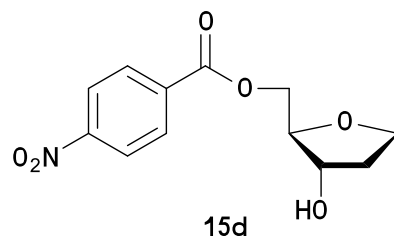
## 5-*O*-*p*-Nitrobenzoyl-1,2-dideoxy-D-ribose (15d)

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75.5 MHz)



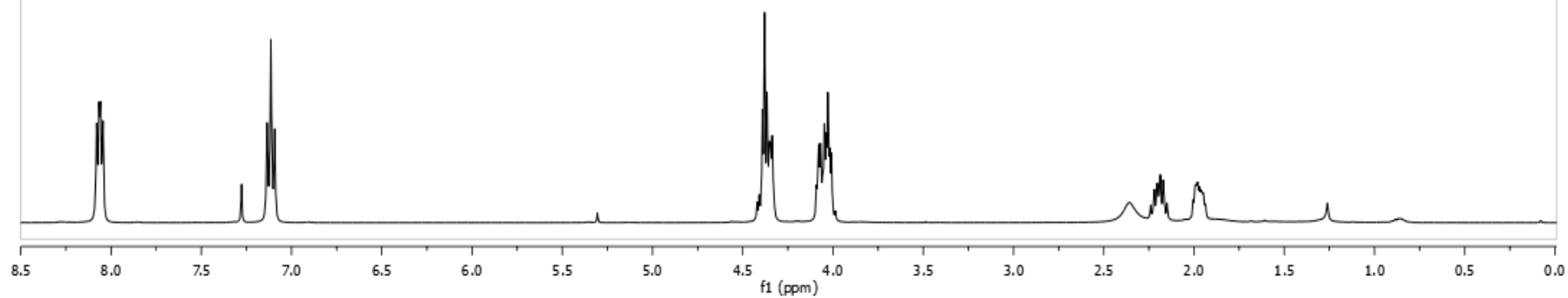
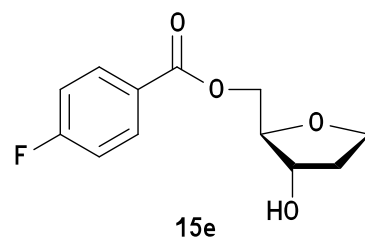
## 5-*O*-*p*-Nitrobenzoyl-1,2-dideoxy-D-ribose (15d)

$^{13}\text{C}$ DEPT NMR ( $\text{CDCl}_3$ , 75.5 MHz)



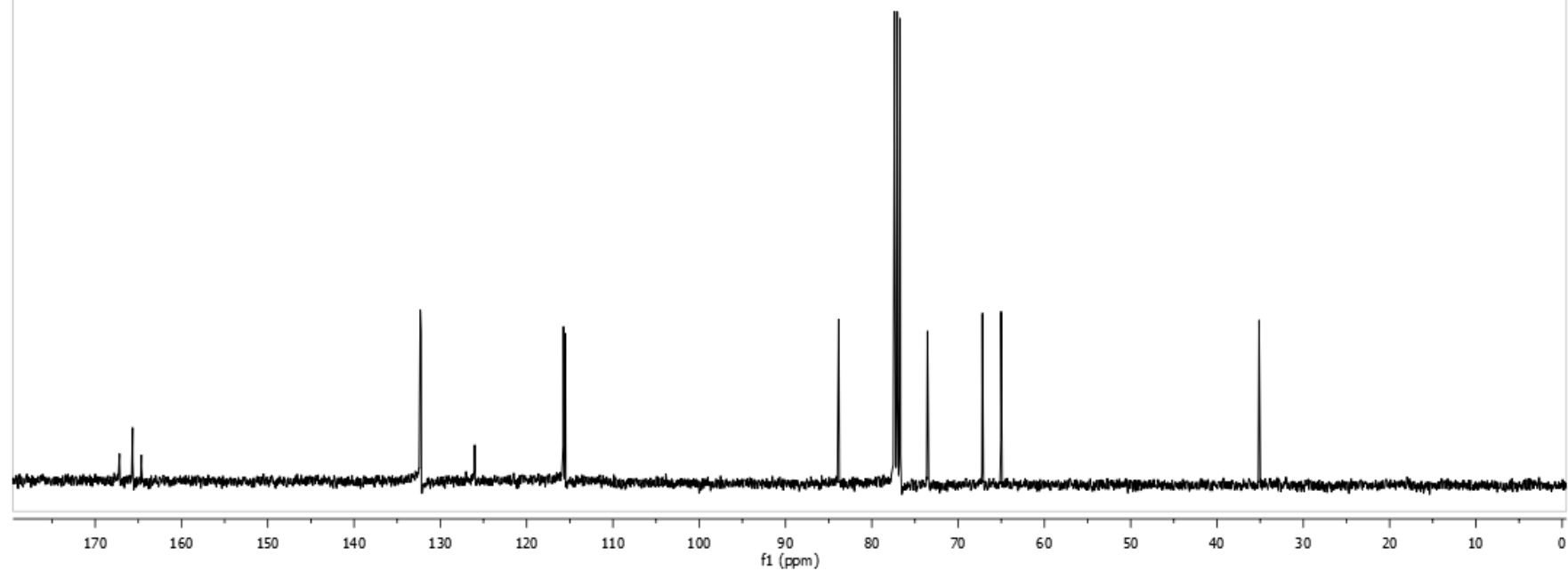
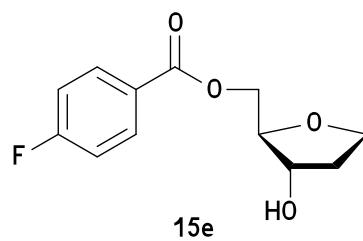
## 5-*O*-*p*-Fluorobenzoyl-1,2-dideoxy-D-ribose (15e)

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400.13)



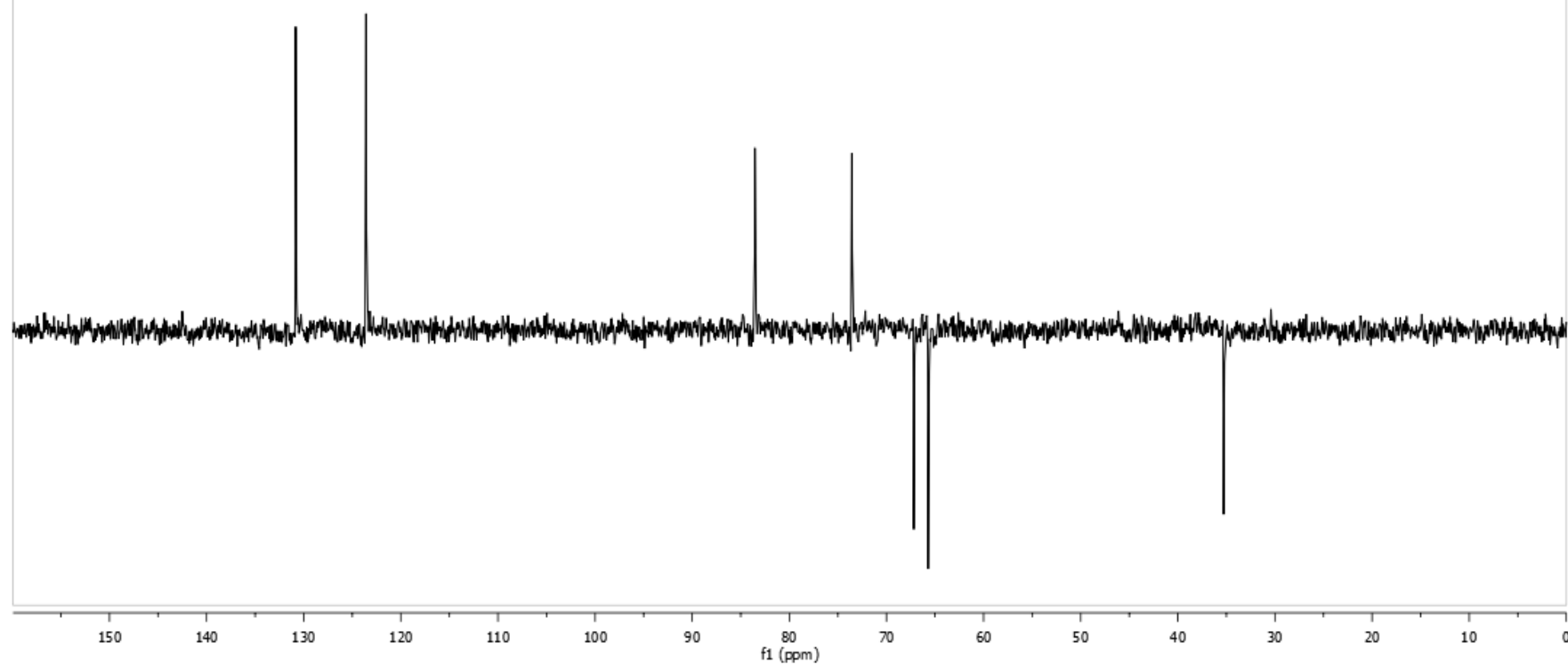
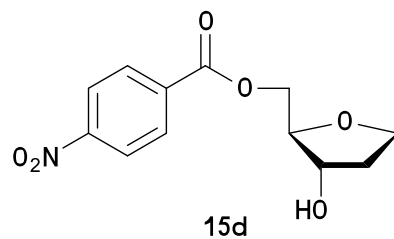
## 5-*O*-*p*-Fluorobenzoyl-1,2-dideoxy-D-ribose (15e)

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100.61 MHz)



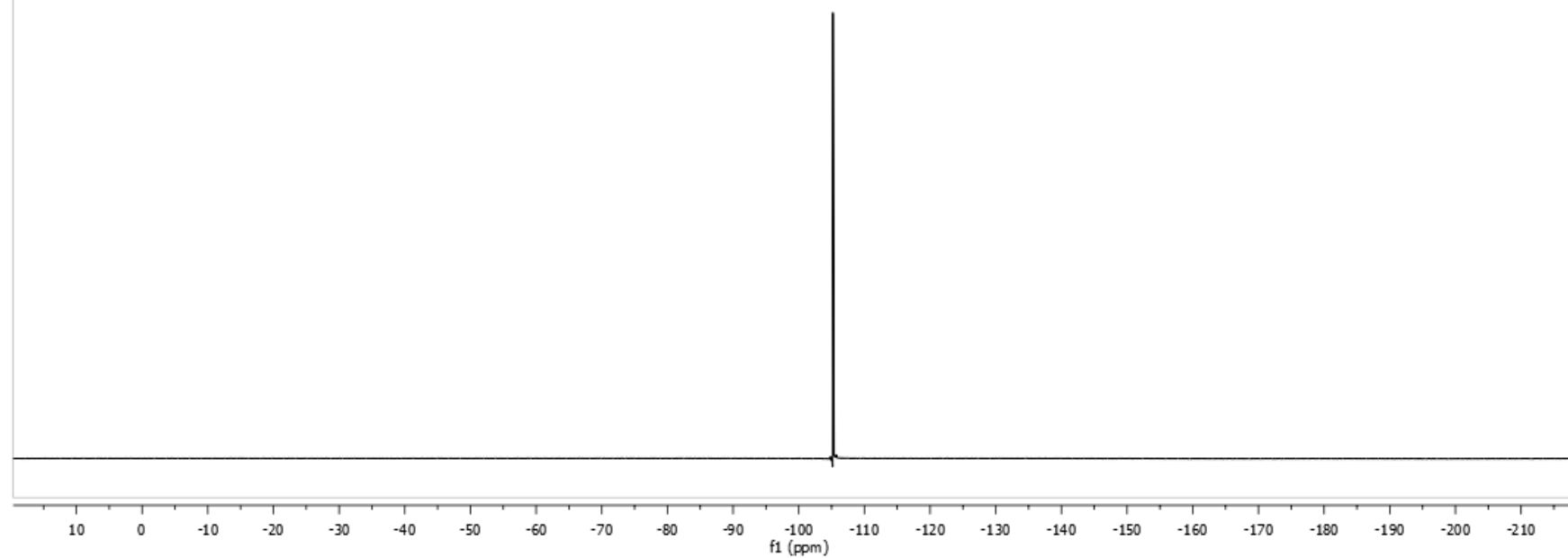
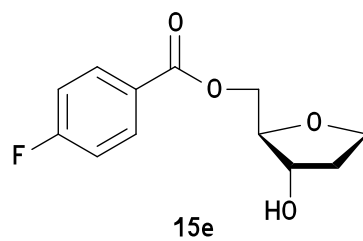
## 5-*O*-*p*-Nitrobenzoyl-1,2-dideoxy-D-ribose (15d)

DEPT NMR ( $\text{CDCl}_3$ , 75.5 MHz)



## 5-*O*-*p*-Fluorobenzoyl-1,2-dideoxy-D-ribose (15e)

$^{19}\text{F}$  NMR ( $\text{CDCl}_3$ , 282 MHz)

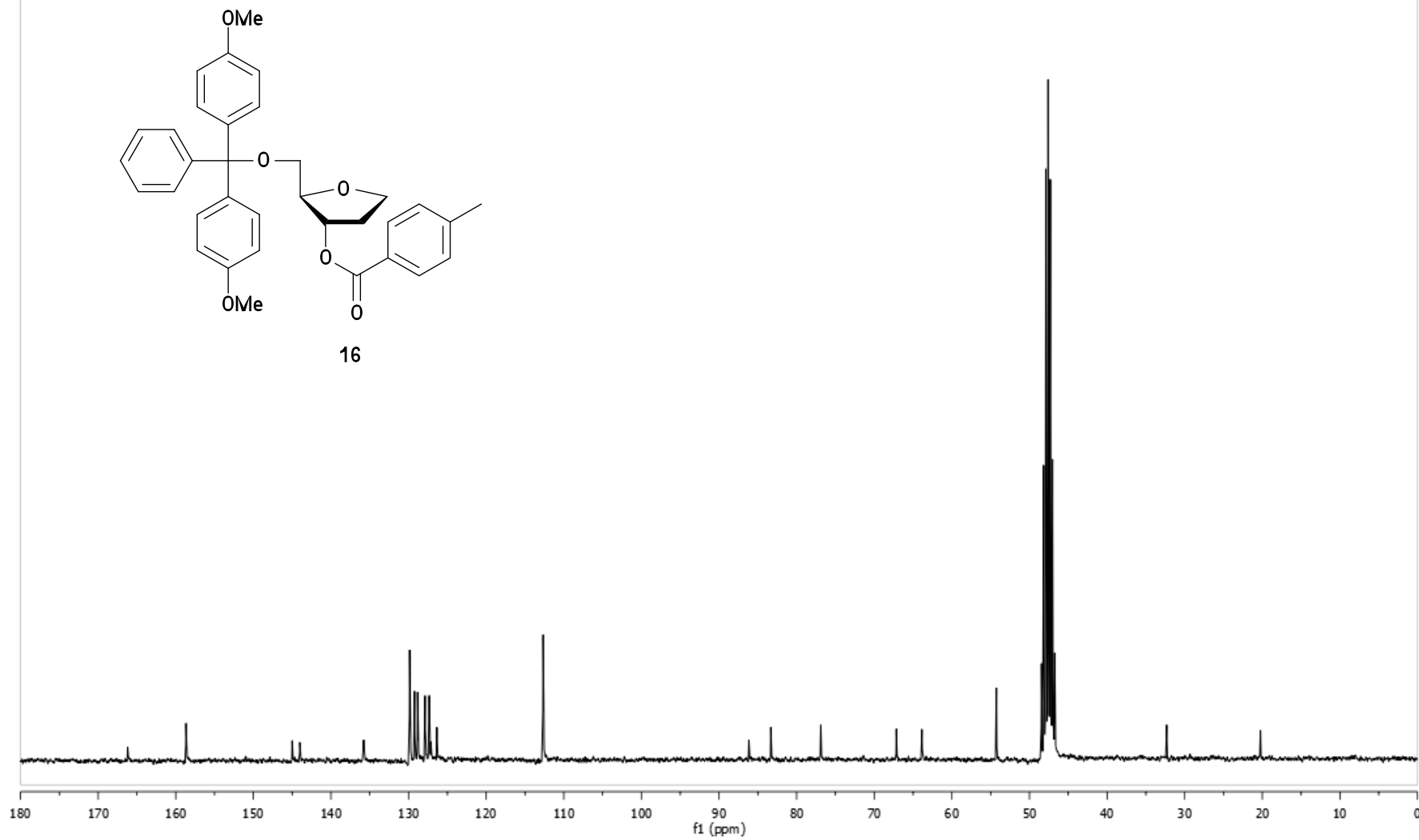


Chemical structure of compound 16: A 4,4'-dimethoxy-1,1'-biphenyl-2,2'-diyl group connected via an ether linkage to a 4-methylphenyl group, which is further connected to a 1,3-dioxolane ring. The 1,3-dioxolane ring is substituted with a 4-methylphenyl group and a carbonyl group.



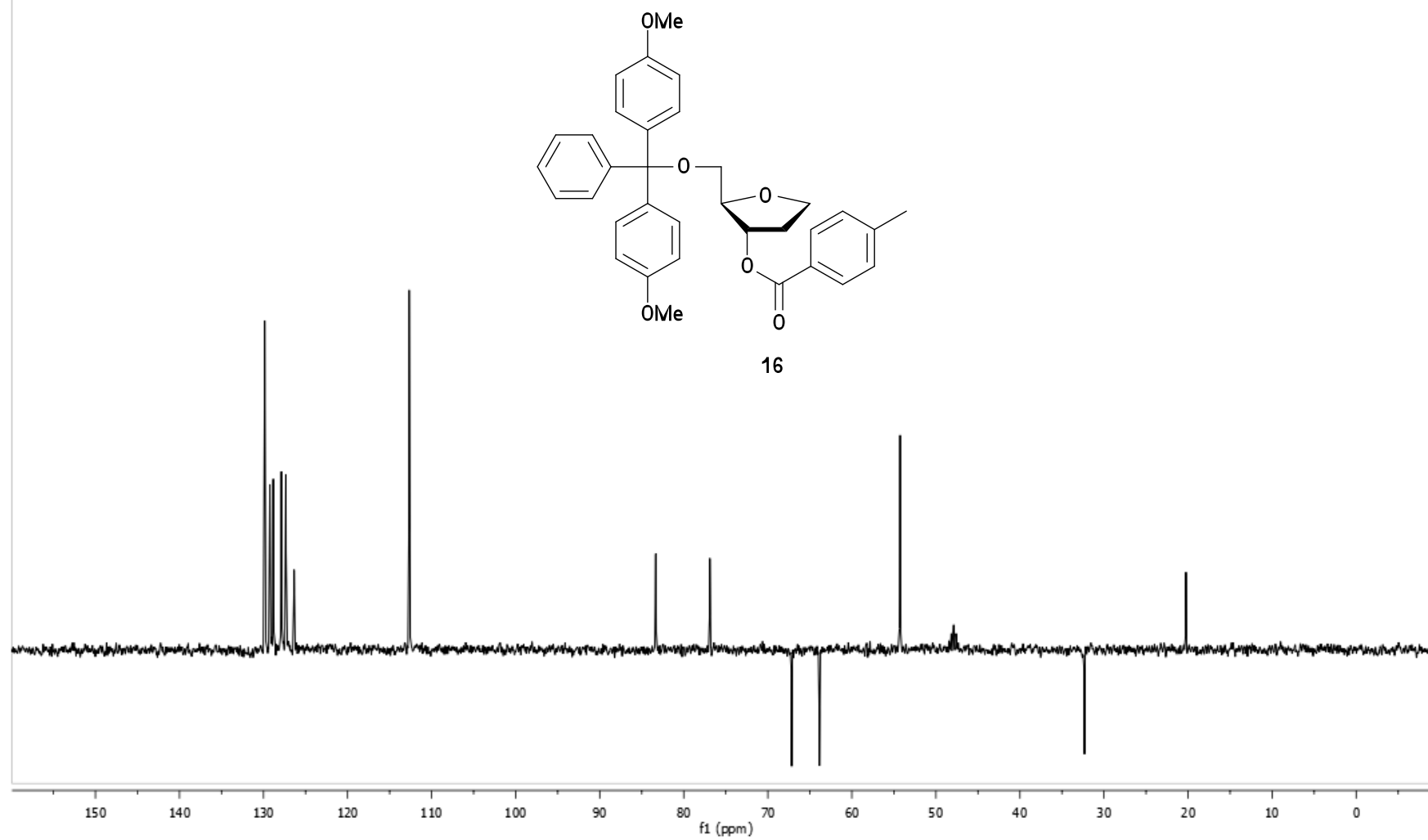
## 5-O-Dimethoxytrityl-3-O-toluoyl-1,2-dideoxy-D-ribose (16)

$^{13}\text{C}$  NMR (MeOH- $d_4$ , 75.5 MHz)



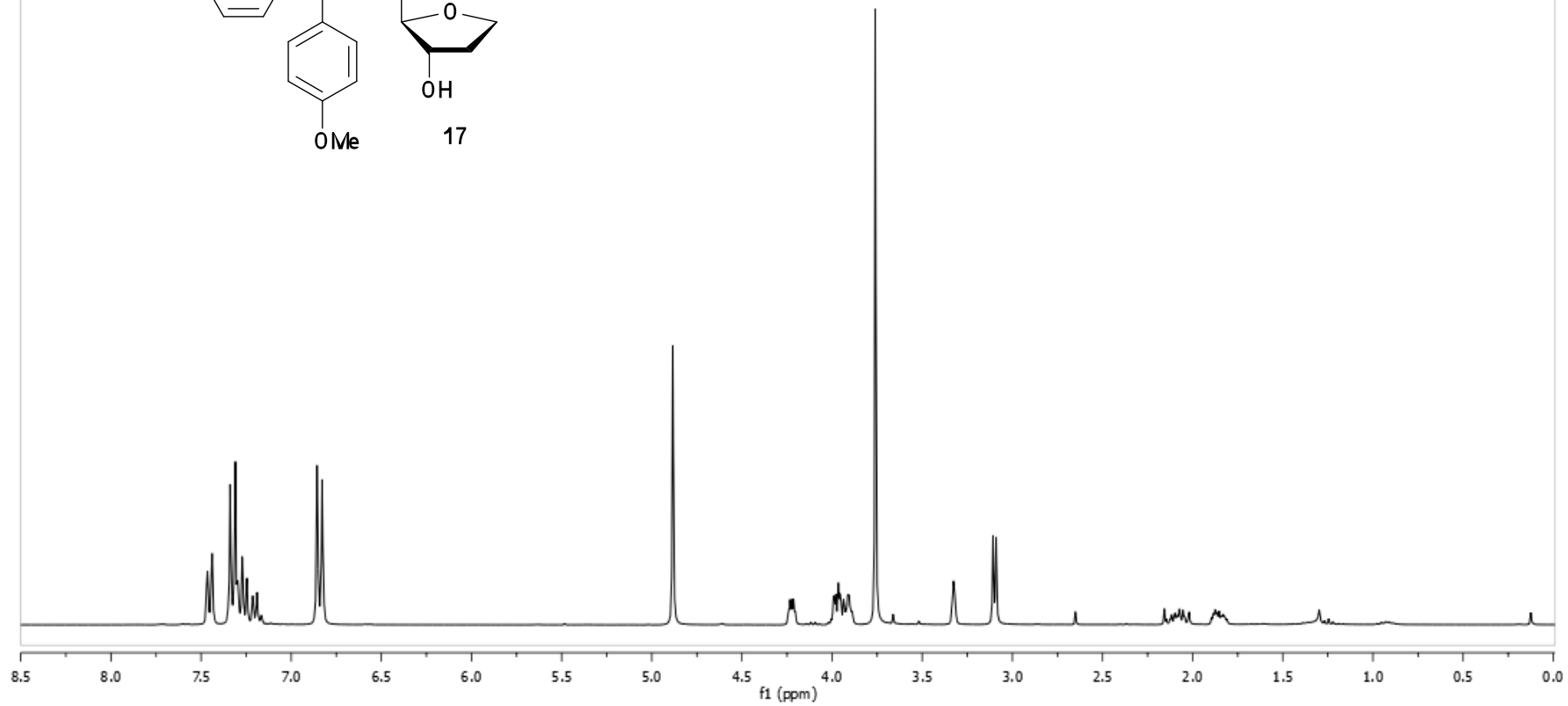
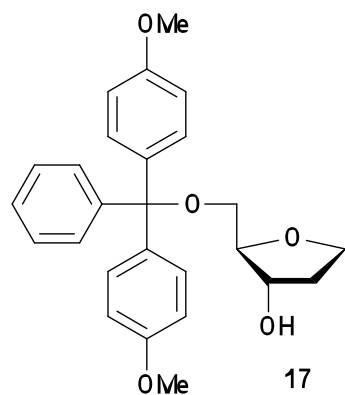
## 5-O-Dimethoxytrityl-3-O-toluoyl-1,2-dideoxy-D-ribose (16)

DEPT NMR (MeOH- $d_4$ , 75.5 MHz)



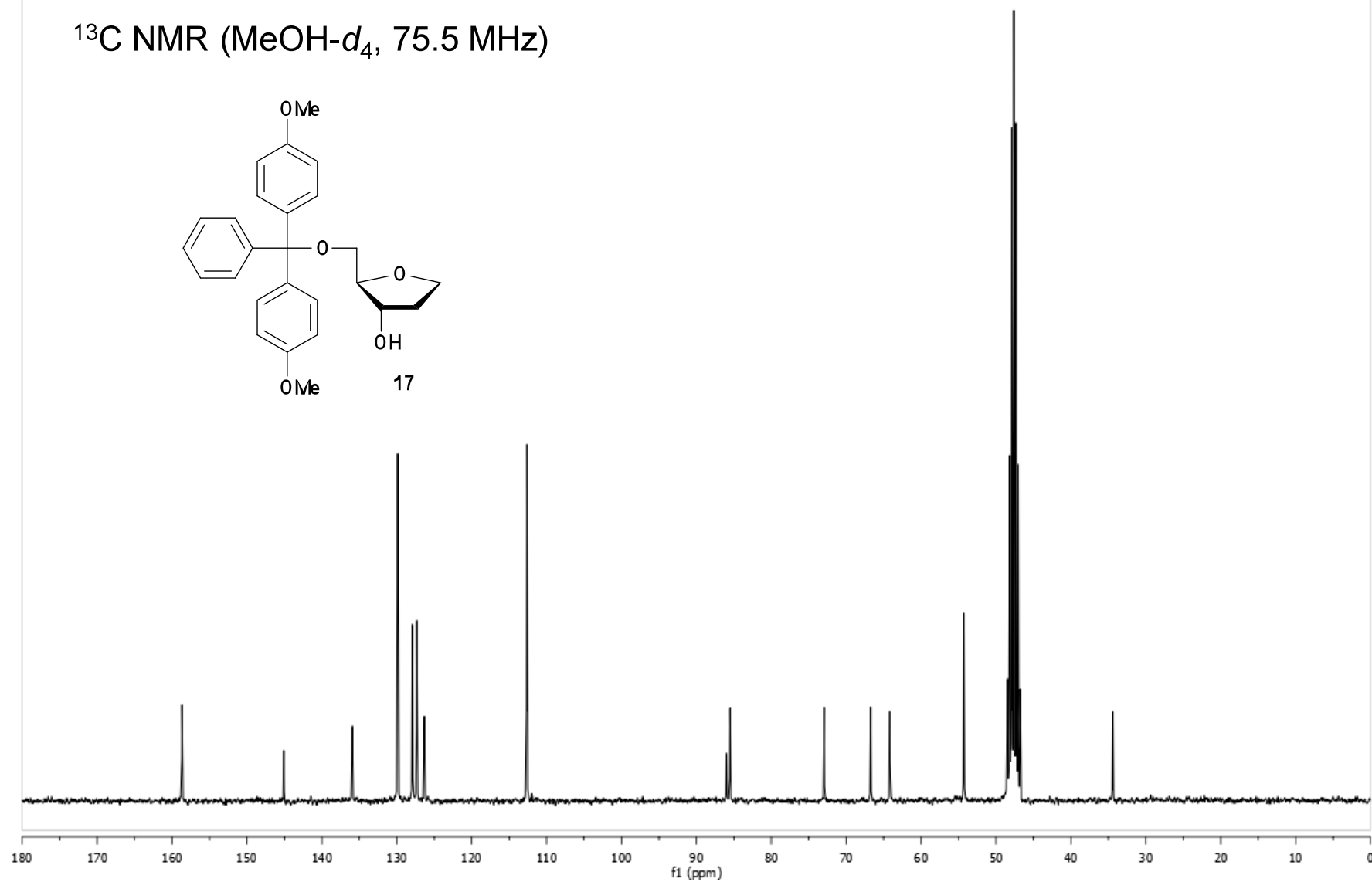
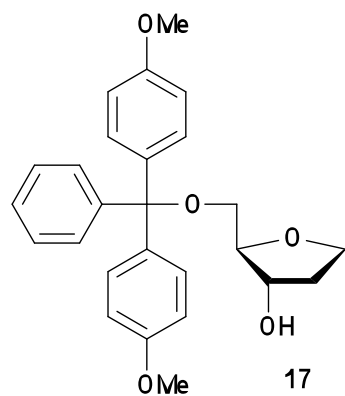
## 5-O-Dimethoxytrityl-1,2-dideoxy-D-ribose (17)

$^1\text{H}$  NMR ( $\text{MeOH-}d_4$ , 300.13 MHz)



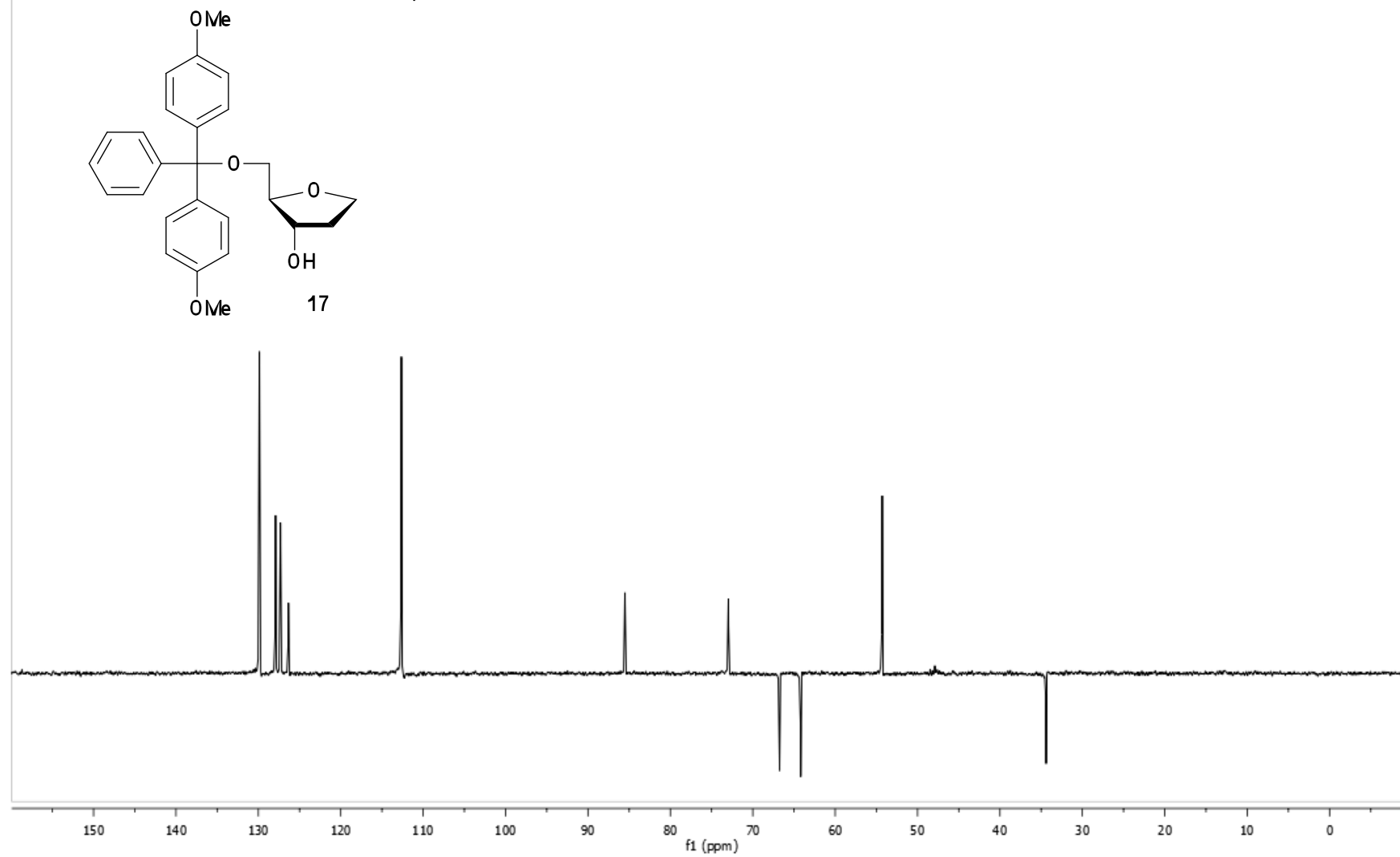
# 5-O-Dimethoxytrityl-1,2-dideoxy-D-ribose (17)

$^{13}\text{C}$  NMR (MeOH- $d_4$ , 75.5 MHz)

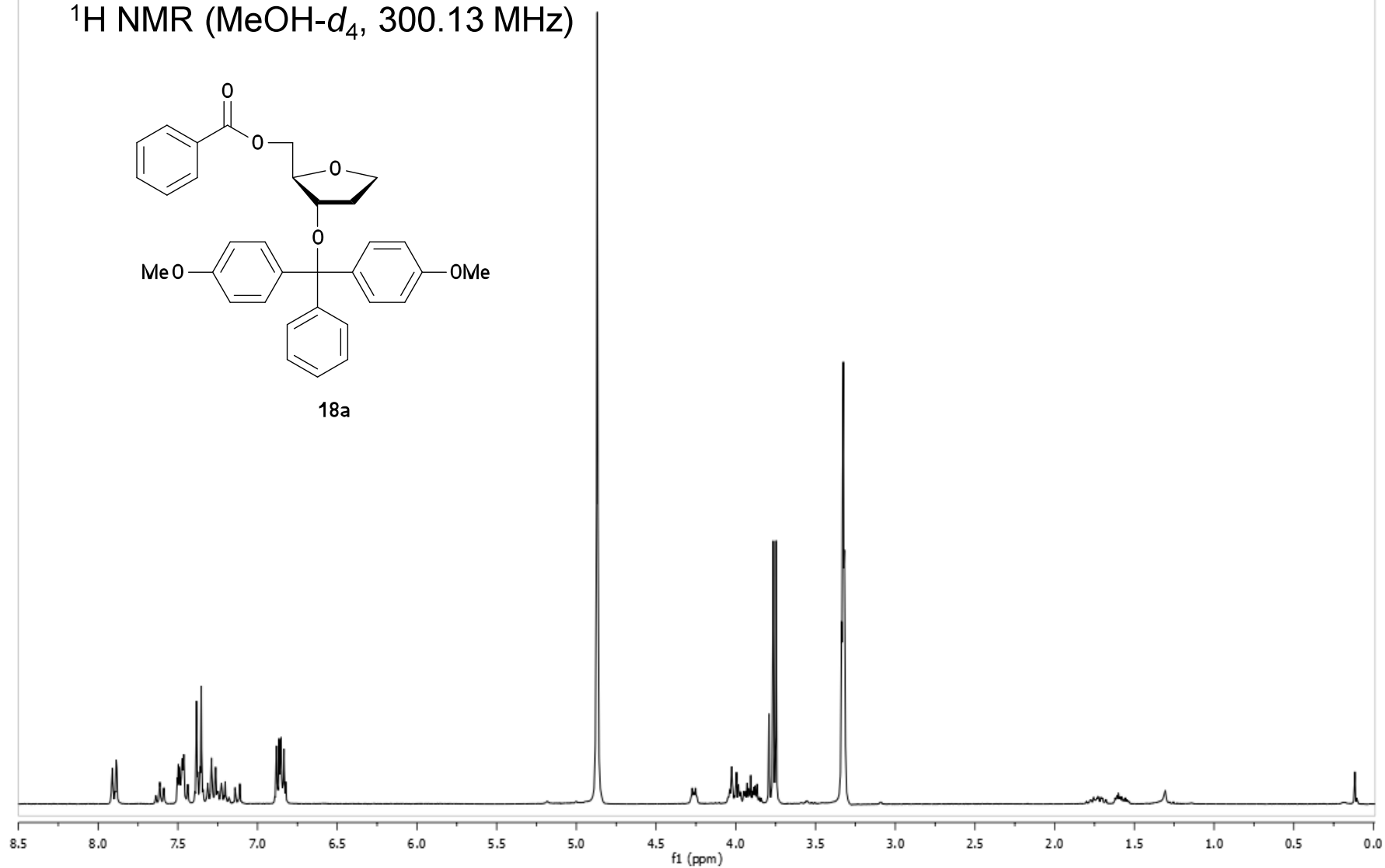


## 5-O-Dimethoxytrityl-1,2-dideoxy-D-ribose (17)

DEPT NMR (MeOH- $d_4$ , 75.5 MHz)

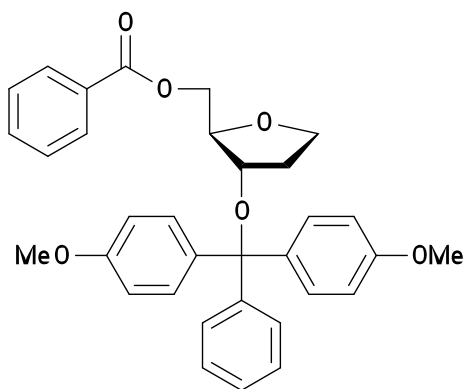


18a

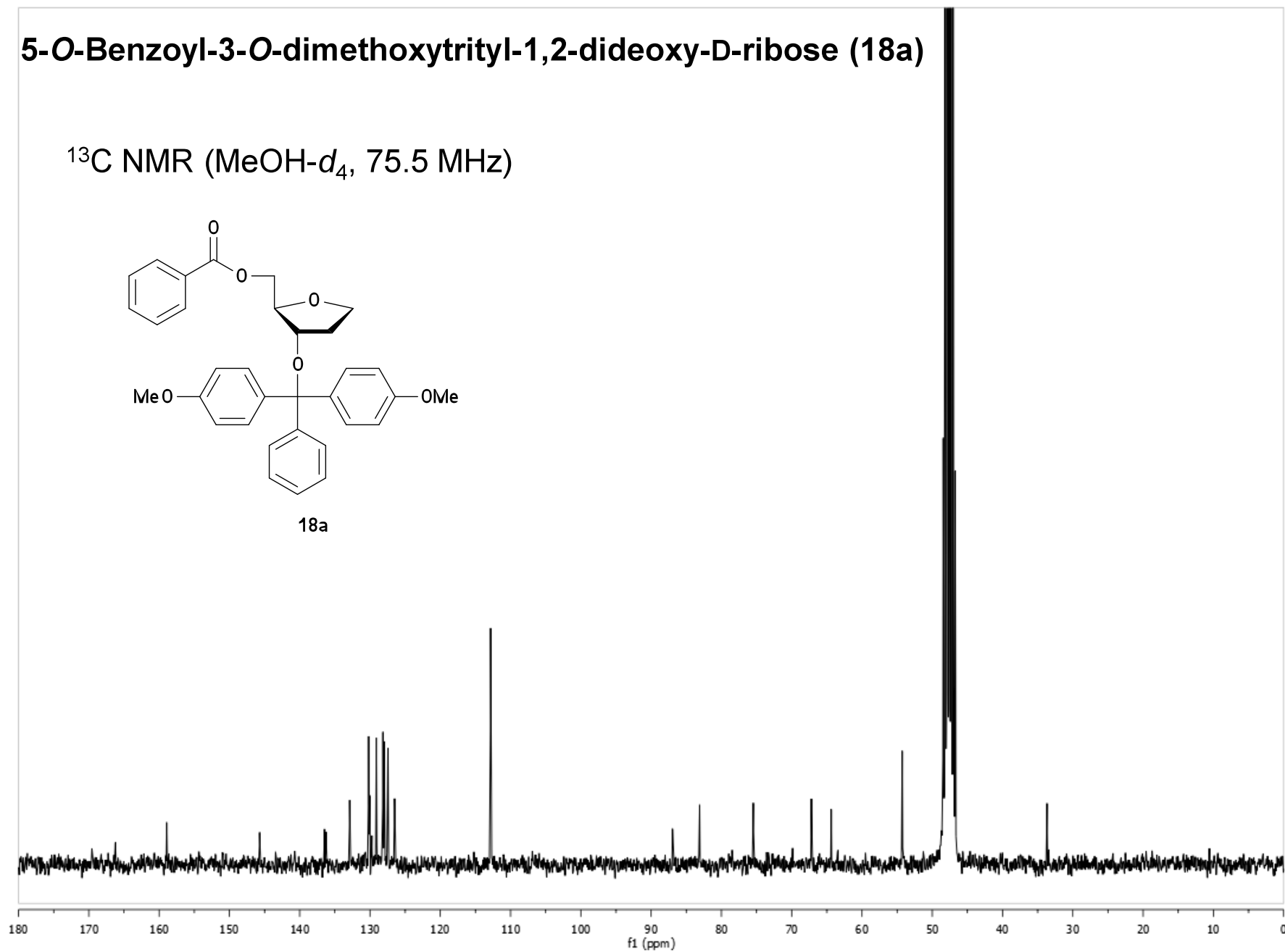


# 5-O-Benzoyl-3-O-dimethoxytrityl-1,2-dideoxy-D-ribose (18a)

$^{13}\text{C}$  NMR (MeOH- $d_4$ , 75.5 MHz)

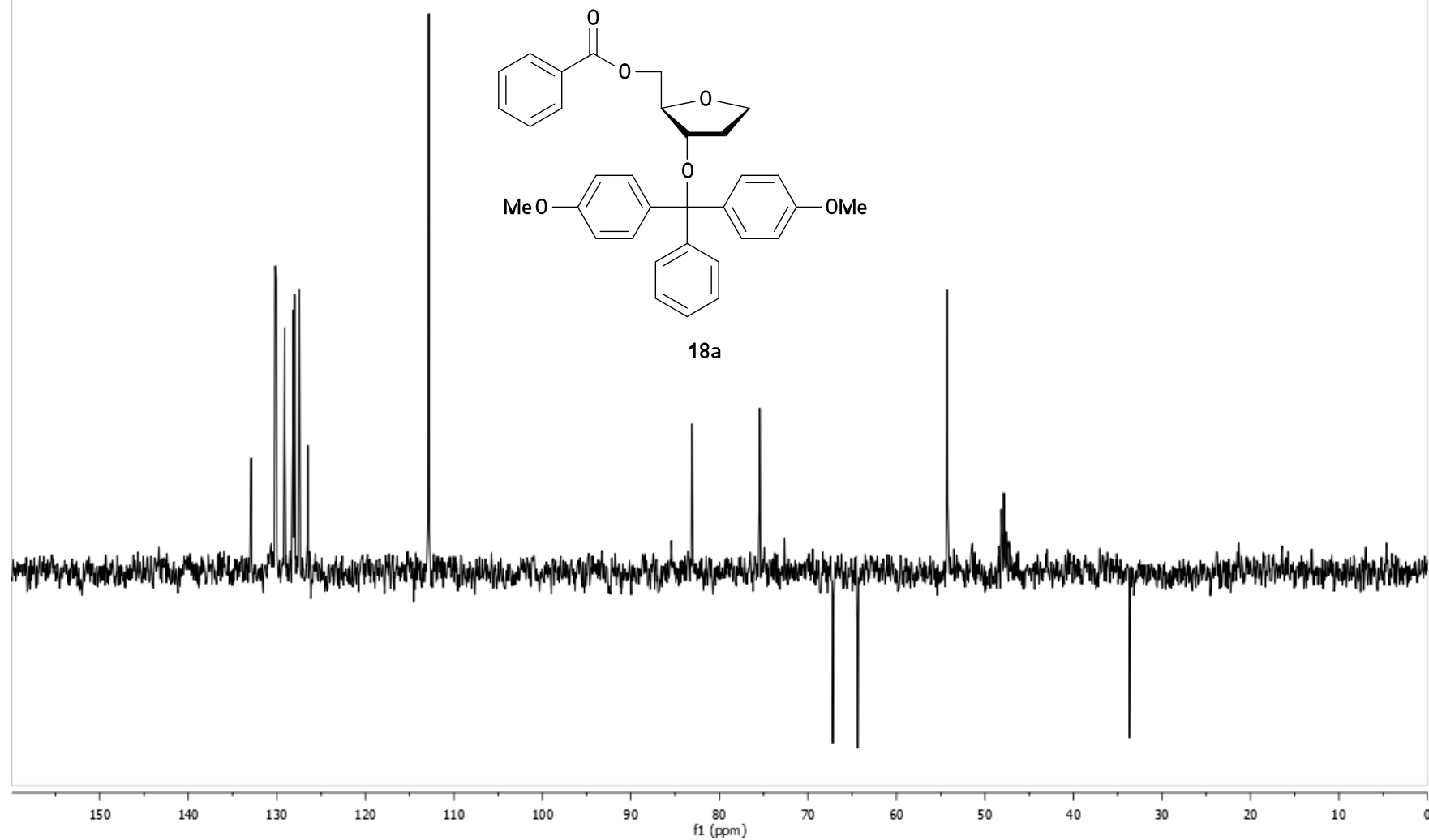


18a



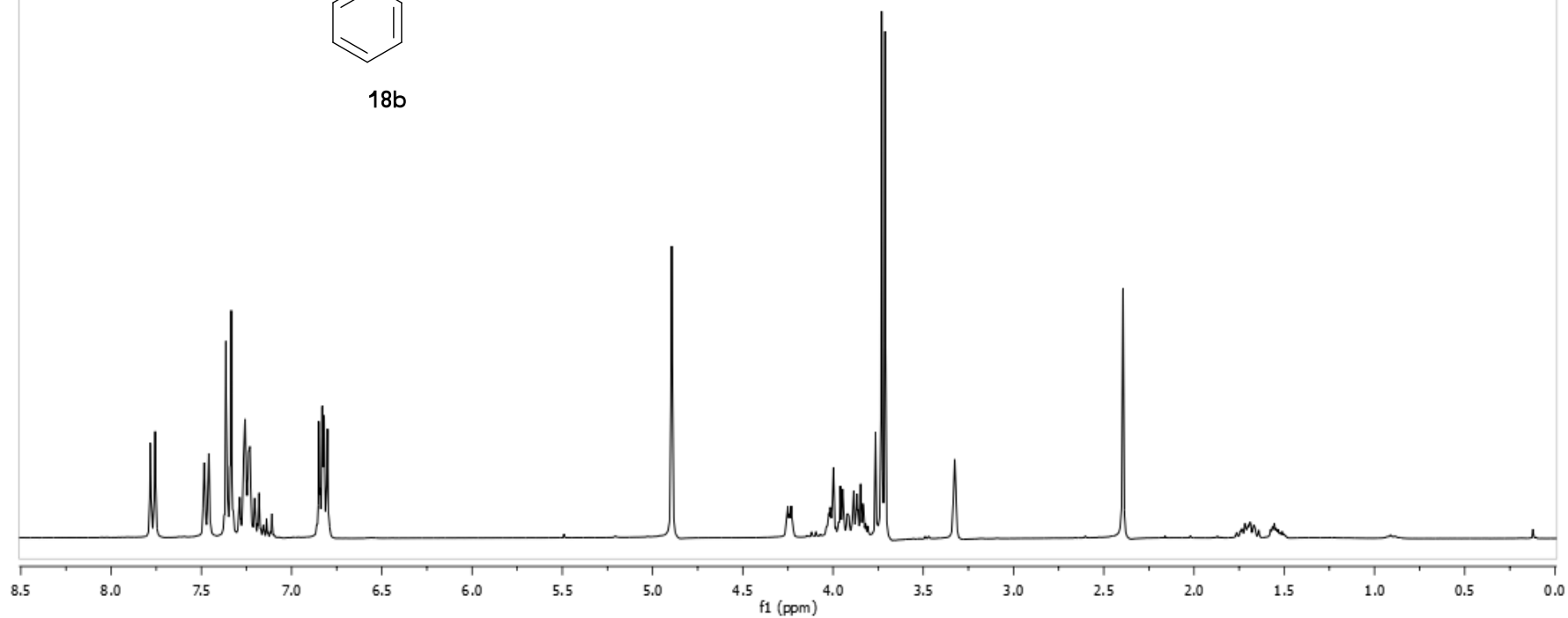
## 5-O-Benzoyl-3-O-dimethoxytrityl-1,2-dideoxy-D-ribose (18a)

DEPT NMR (MeOH- $d_4$ , 75.5 MHz)



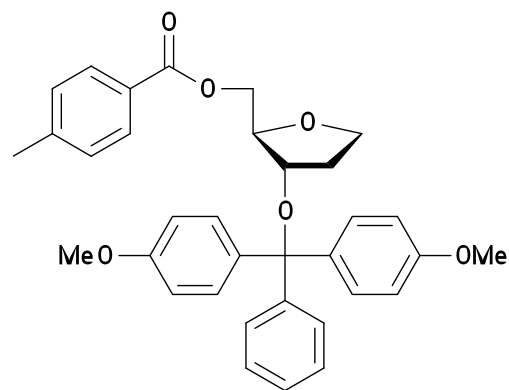
The chemical structure shows a central quaternary carbon atom bonded to four different groups: an unsubstituted phenyl ring, two 4-methoxyphenyl rings, and a tetrahydropyran ring. The tetrahydropyran ring is substituted at the 2-position with a p-methylbenzoate group (-CH<sub>2</sub>-C(=O)-C<sub>6</sub>H<sub>4</sub>-CH<sub>3</sub>). The oxygen atoms are shown as 'O'.

18b

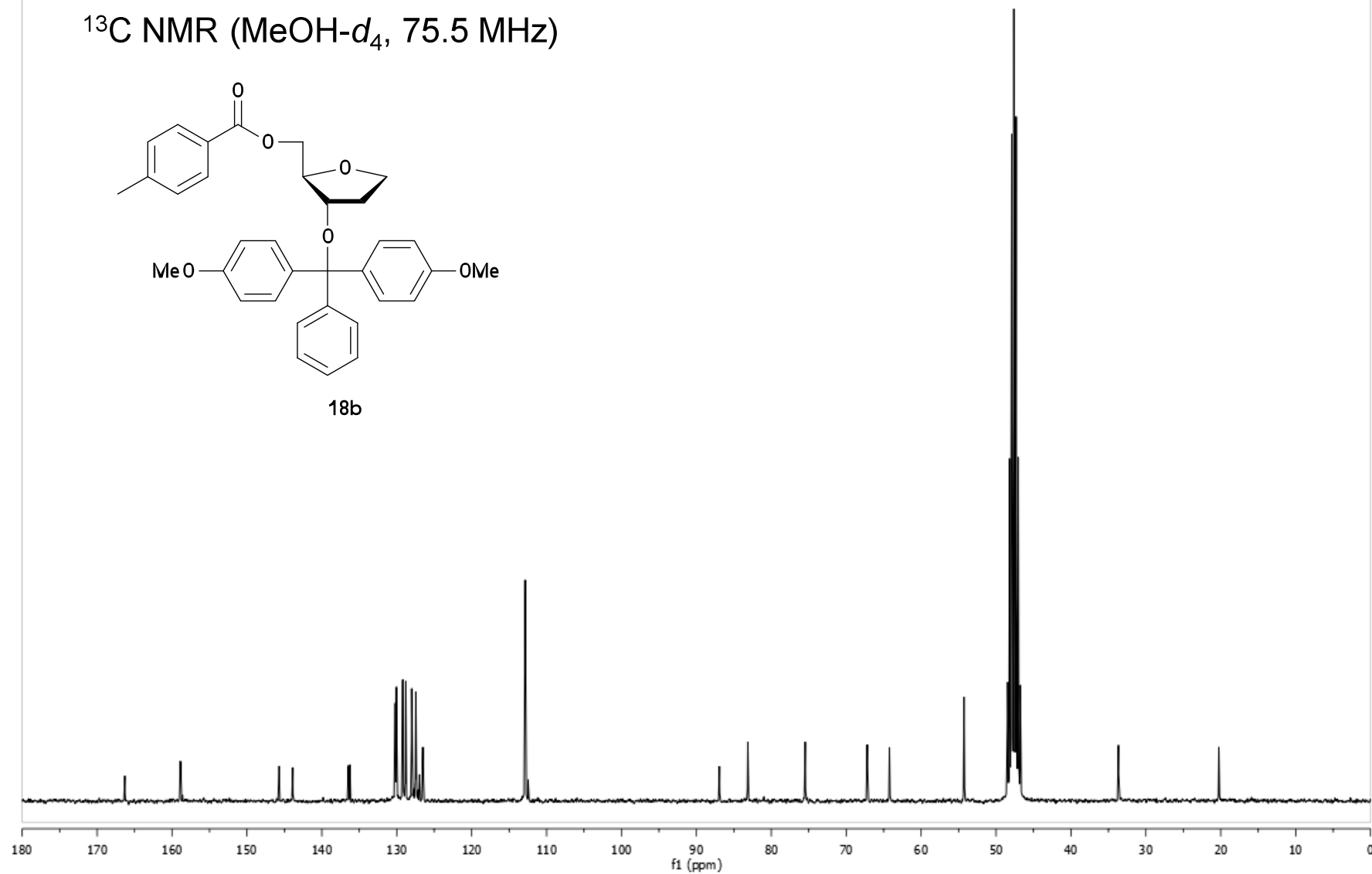


# 3-*O*-Dimethoxytrityl-5-*O*-toluoyl-1,2-dideoxy-D-ribose (18b)

$^{13}\text{C}$  NMR (MeOH- $d_4$ , 75.5 MHz)

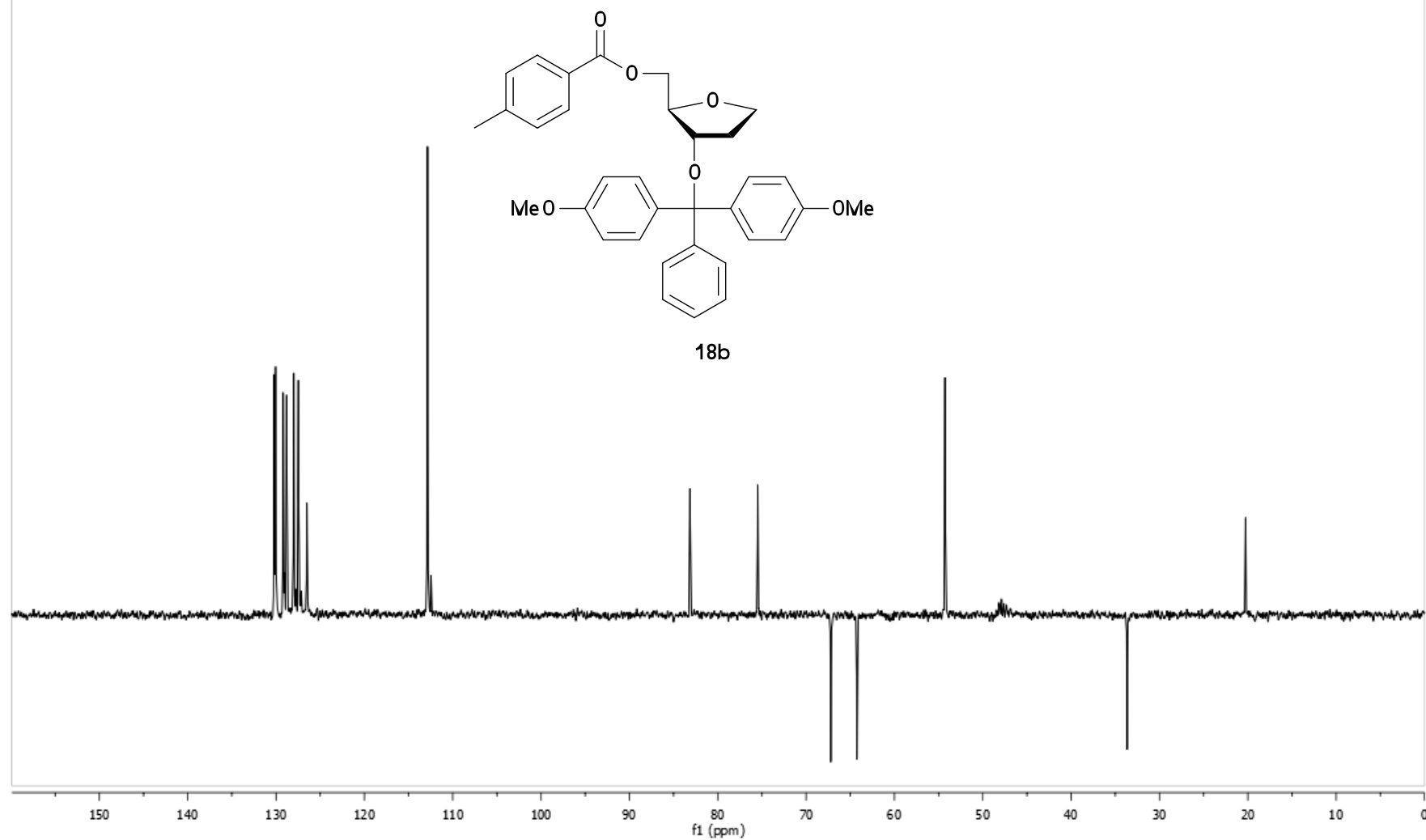


18b



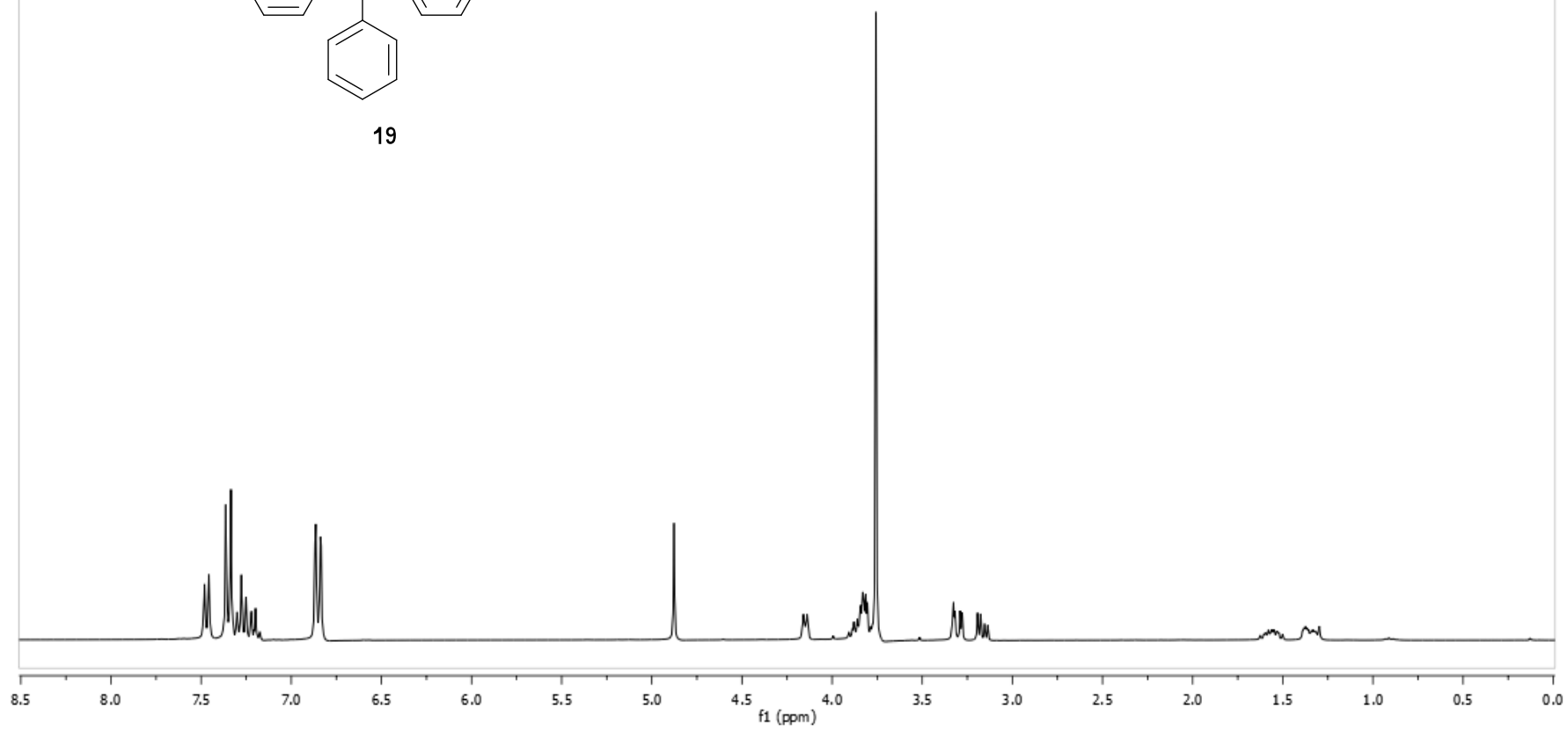
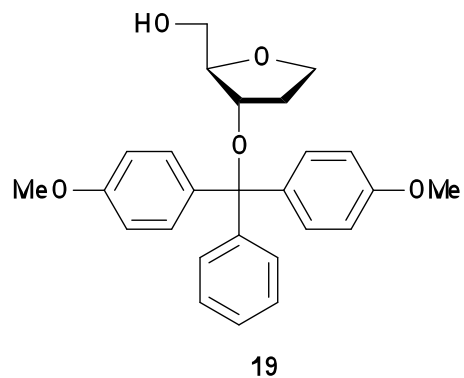
## 3-O-Dimethoxytrityl-5-O-toluoyl-1,2-dideoxy-D-ribose (18b)

DEPT NMR (MeOH- $d_4$ , 75.5 MHz)



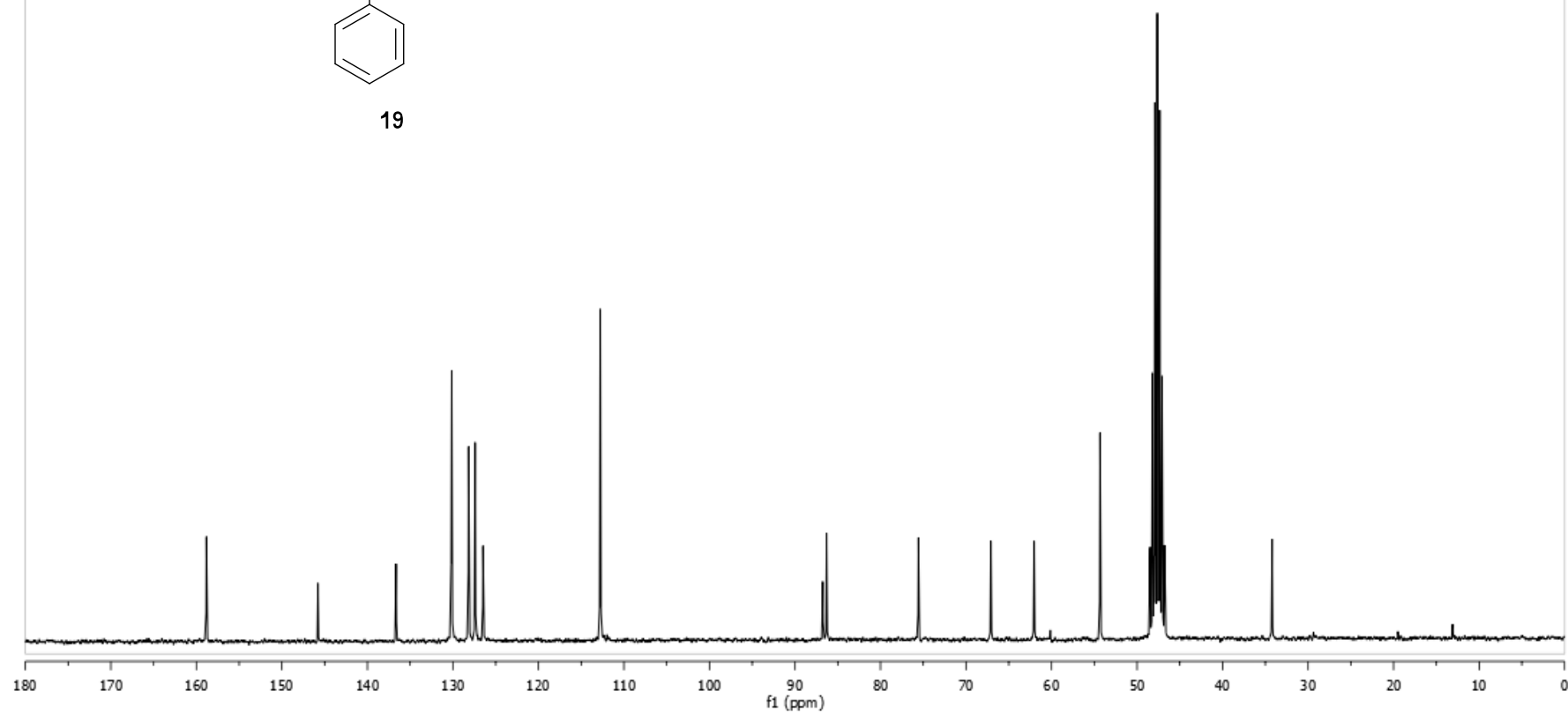
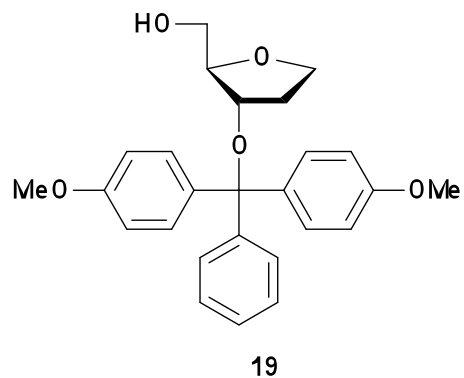
### 3-*O*-Dimethoxytrityl-1,2-dideoxy-D-ribose (19)

$^1\text{H}$  NMR (MeOH- $d_4$ , 300.13 MHz)



### 3-O-Dimethoxytrityl-1,2-dideoxy-D-ribose (19)

$^{13}\text{C}$  NMR (MeOH- $d_4$ , 75.5 MHz)



### 3-O-Dimethoxytrityl-1,2-dideoxy-D-ribose (19)

DEPT NMR (MeOH- $d_4$ , 75.5 MHz)

