

# New MraY<sub>AA</sub> Inhibitors with an Aminoribosyl Uridine Structure and an Oxadiazole

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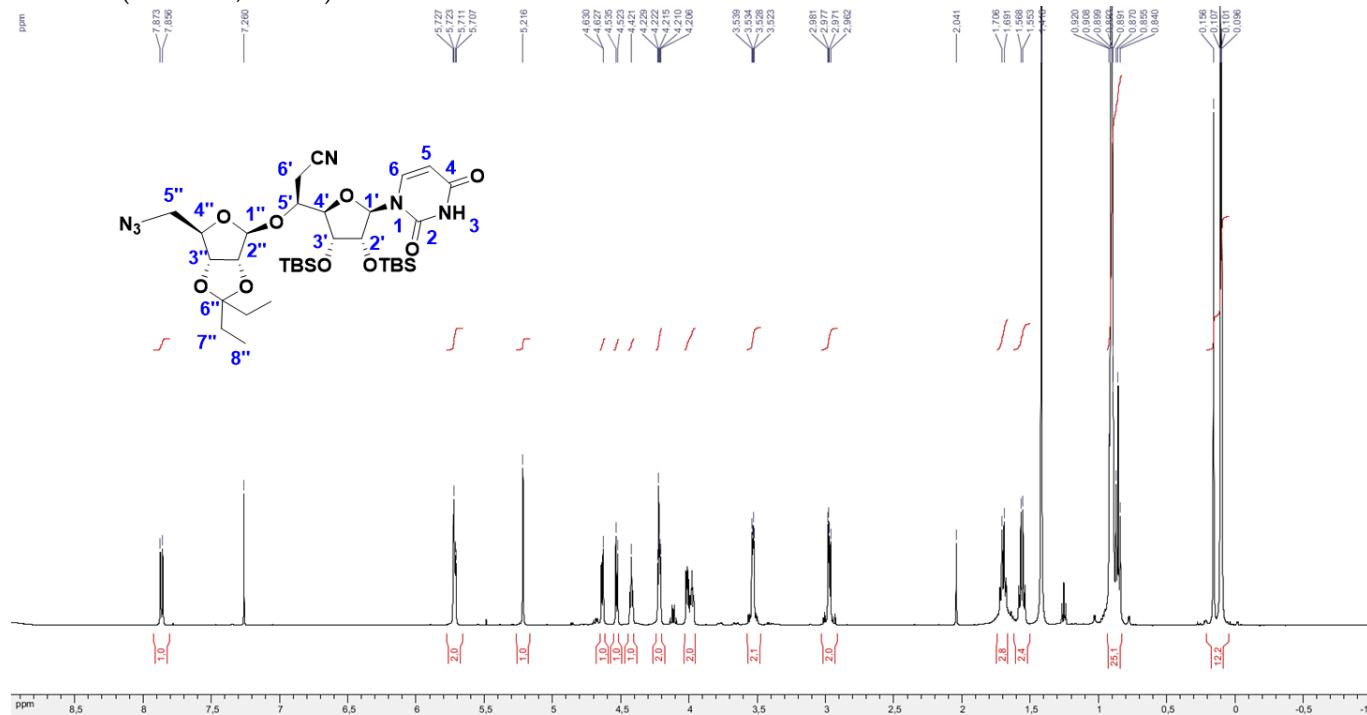
## ELECTRONIC SUPPLEMENTARY MATERIAL

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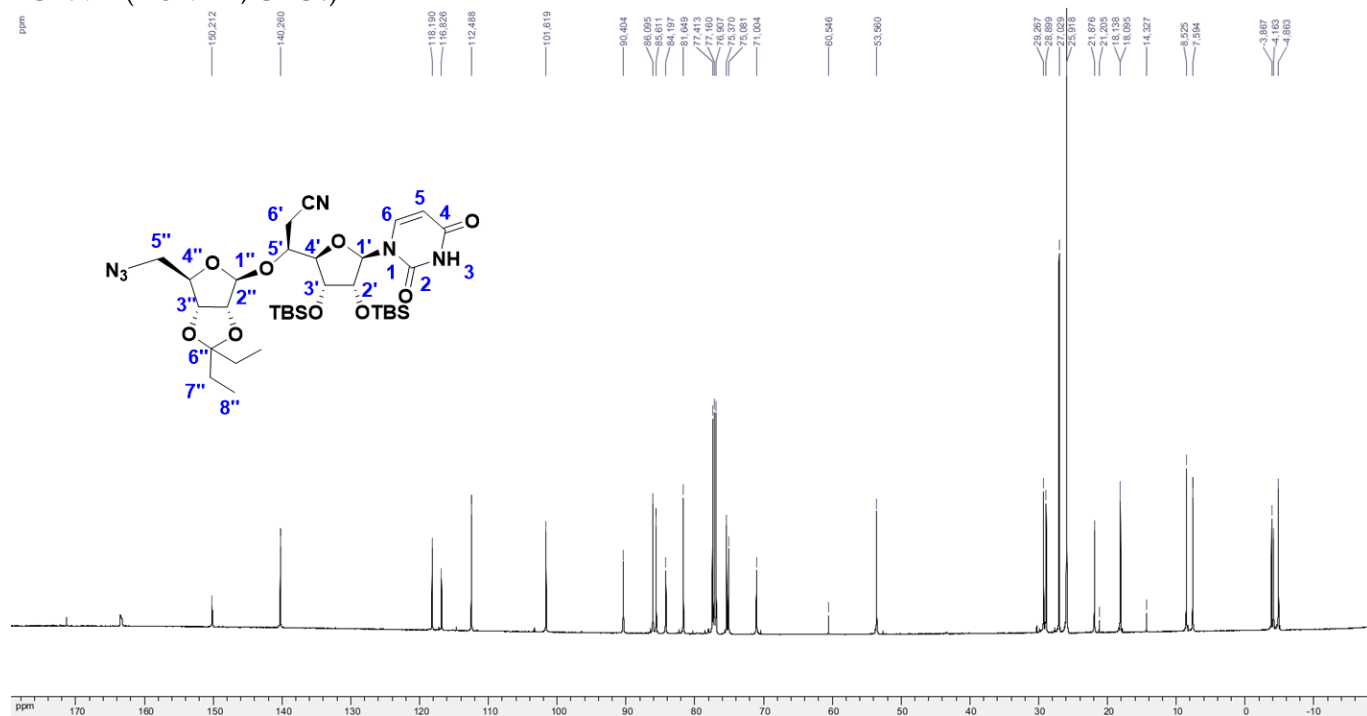
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# Protected Nitrile 1

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

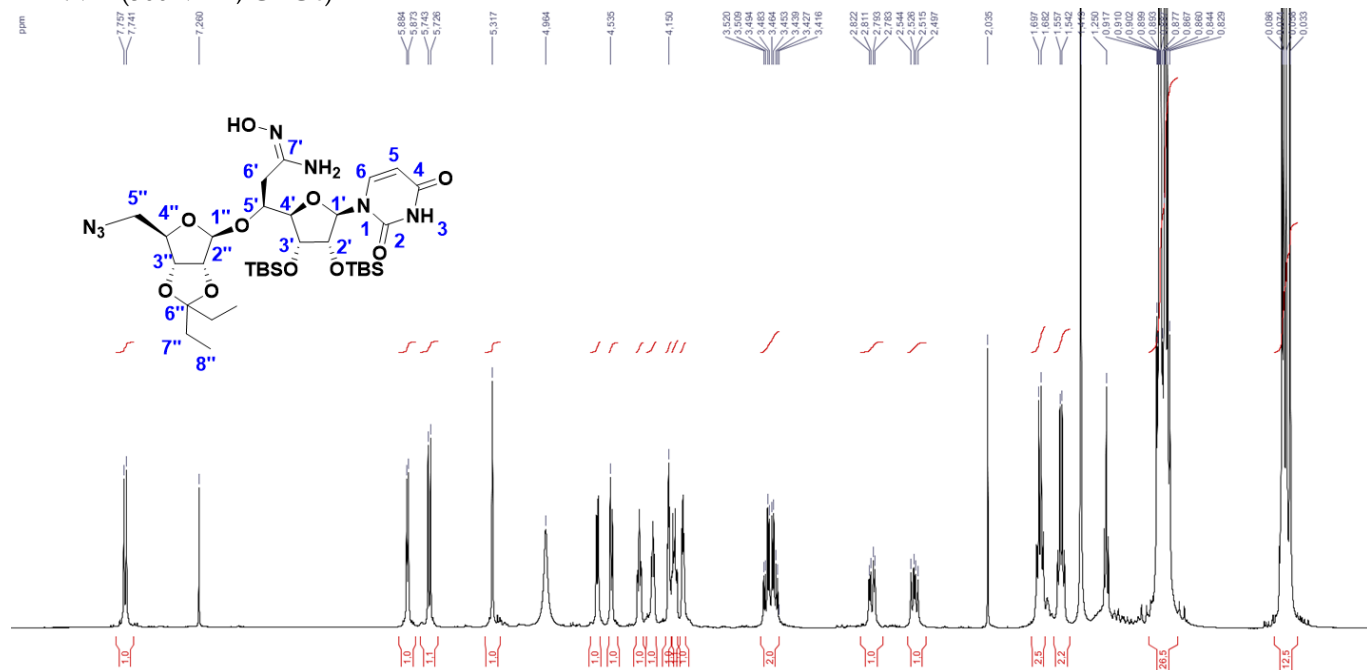


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )

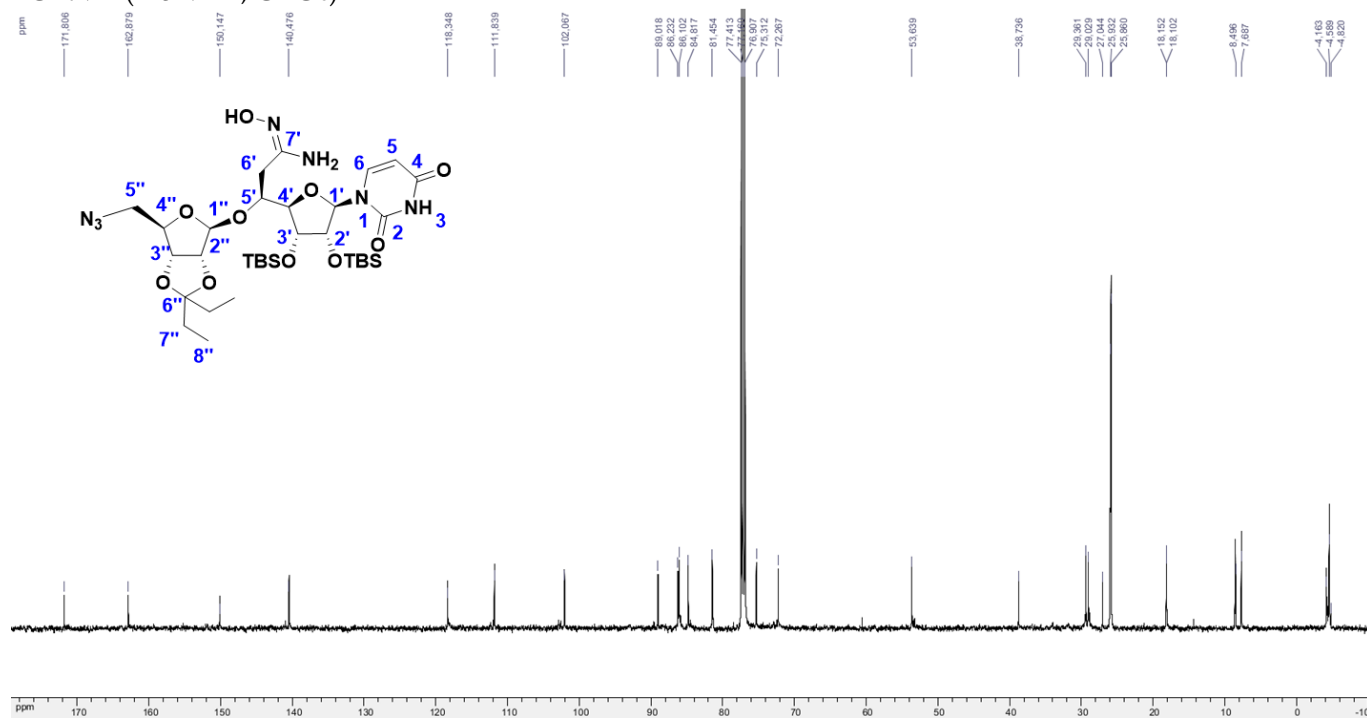


# Protected Amidoxime 2

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)

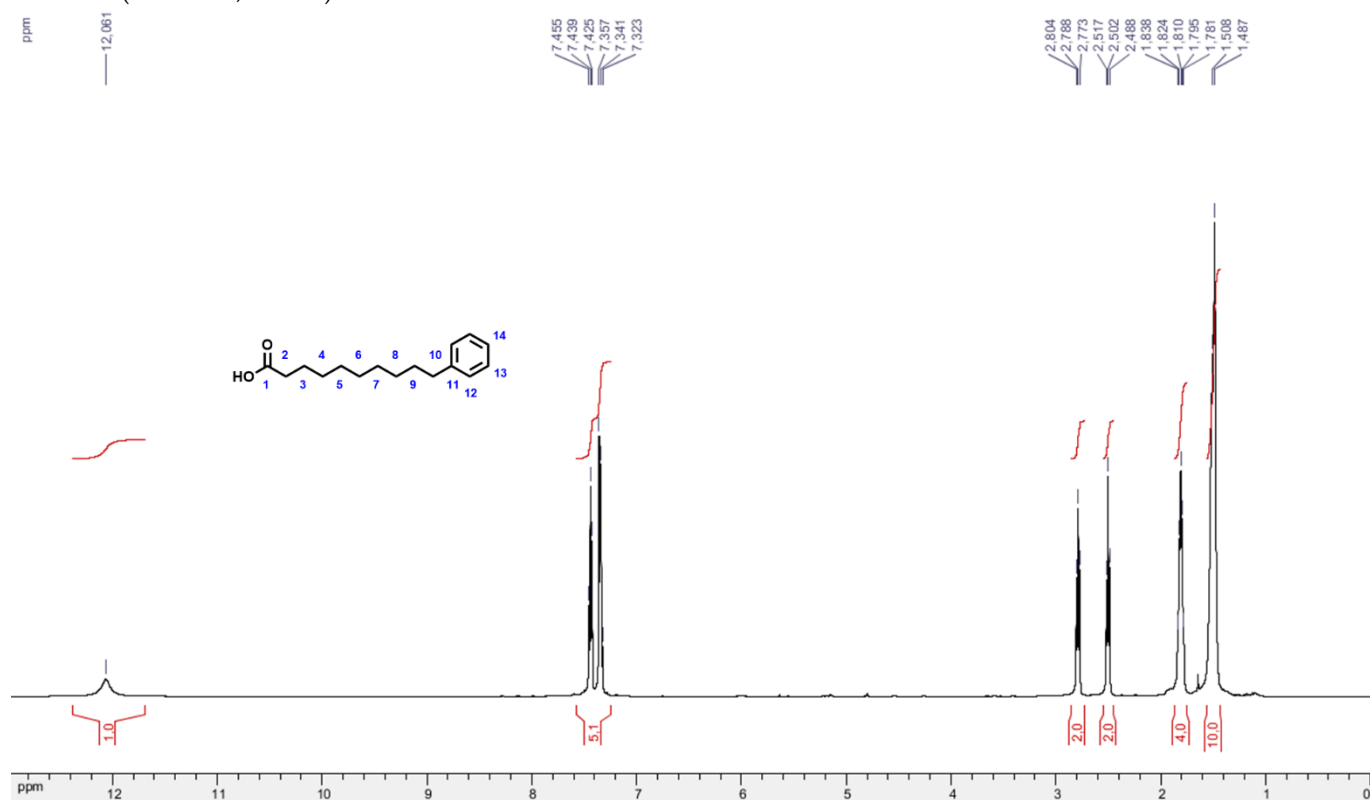


<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)



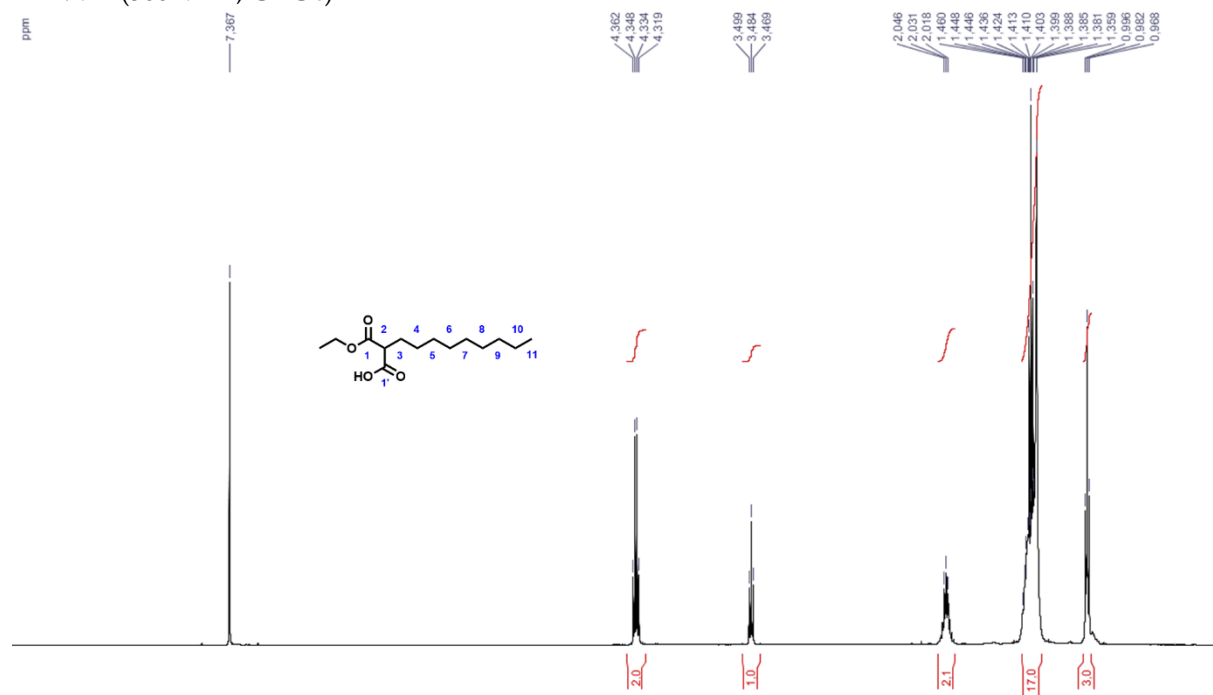
# 10-phenyldecanoic acid 4

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

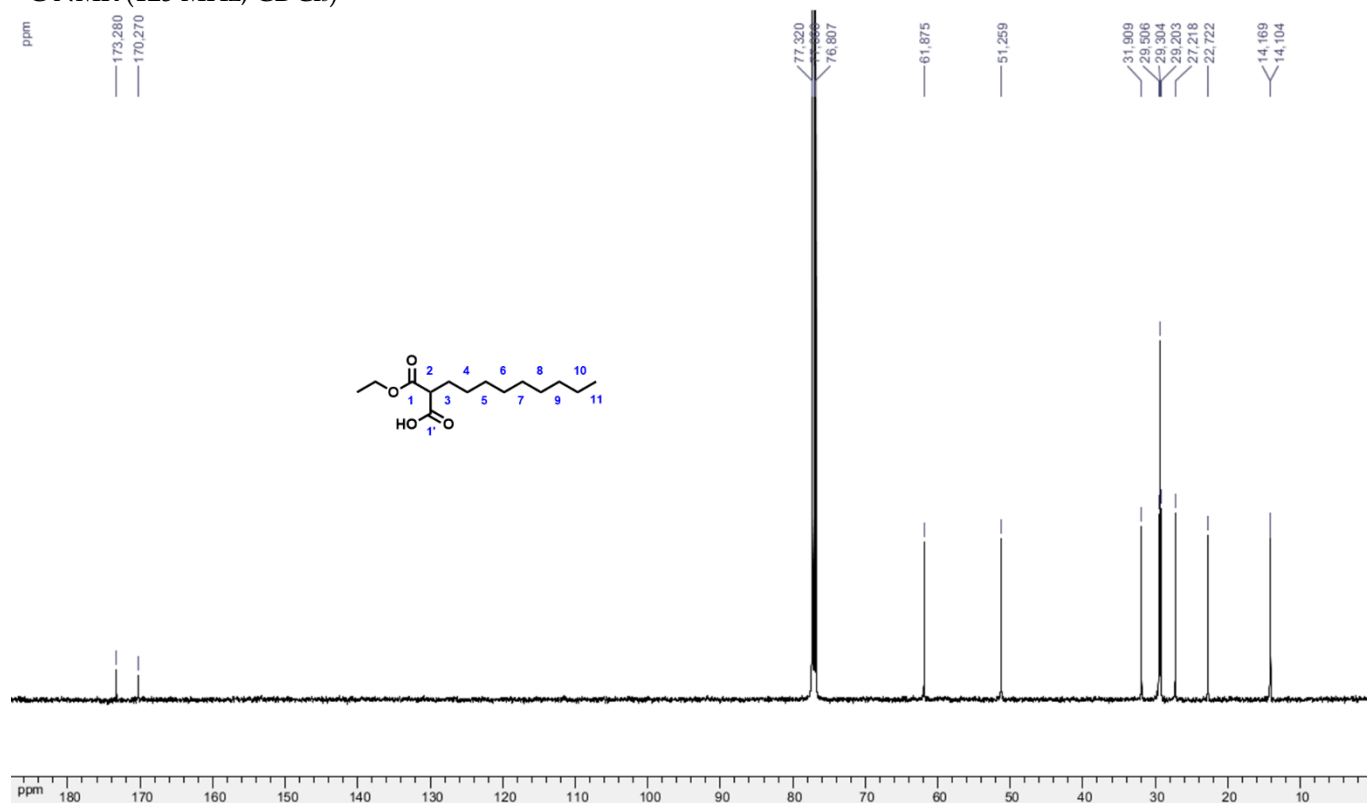


# 2-(Ethoxycarbonyl)undecanoic acid 6

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

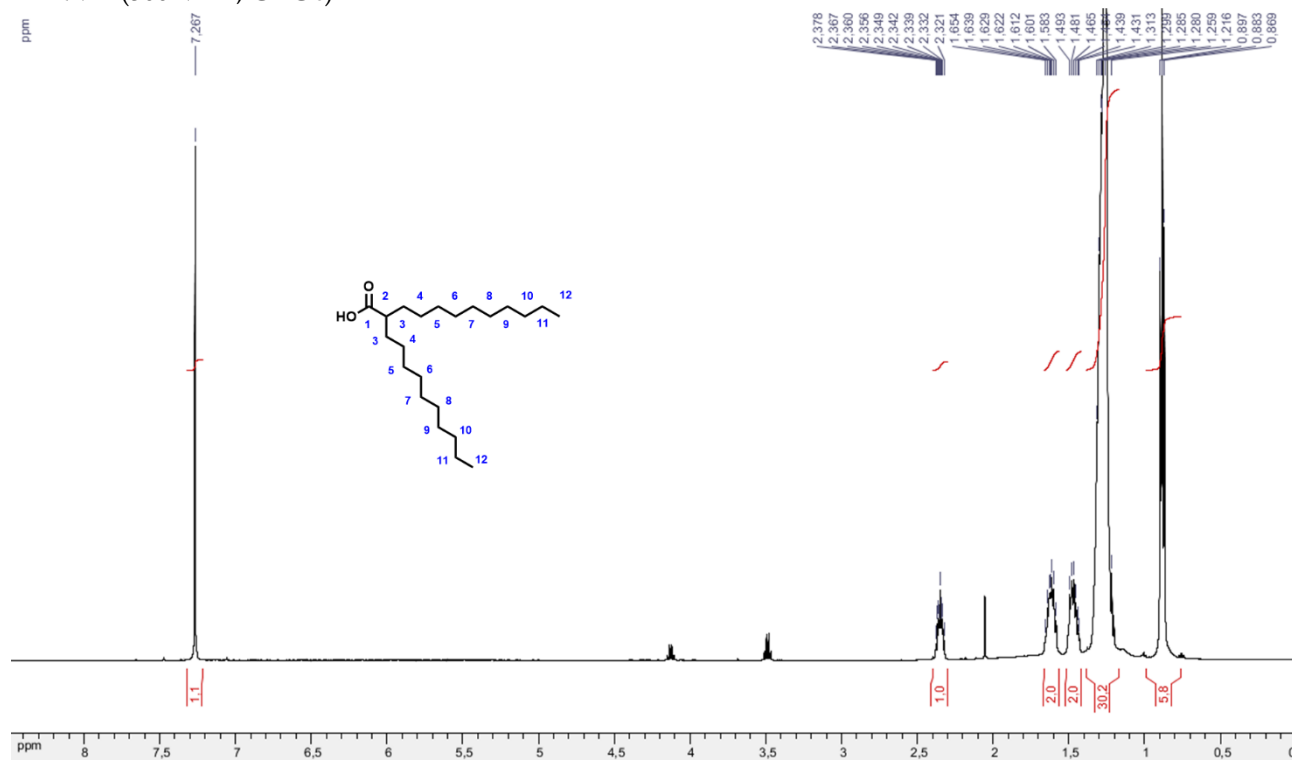


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )

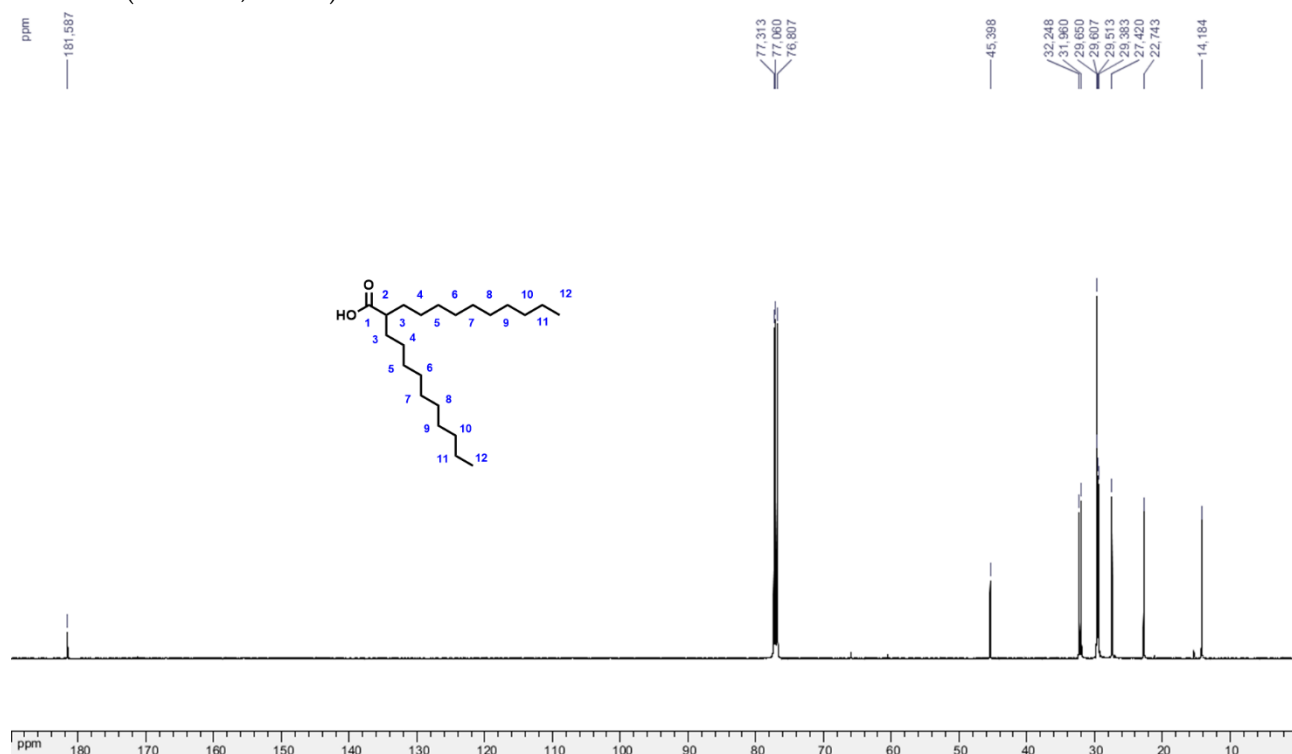


# 2-Decyldodecanoic acid 9

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

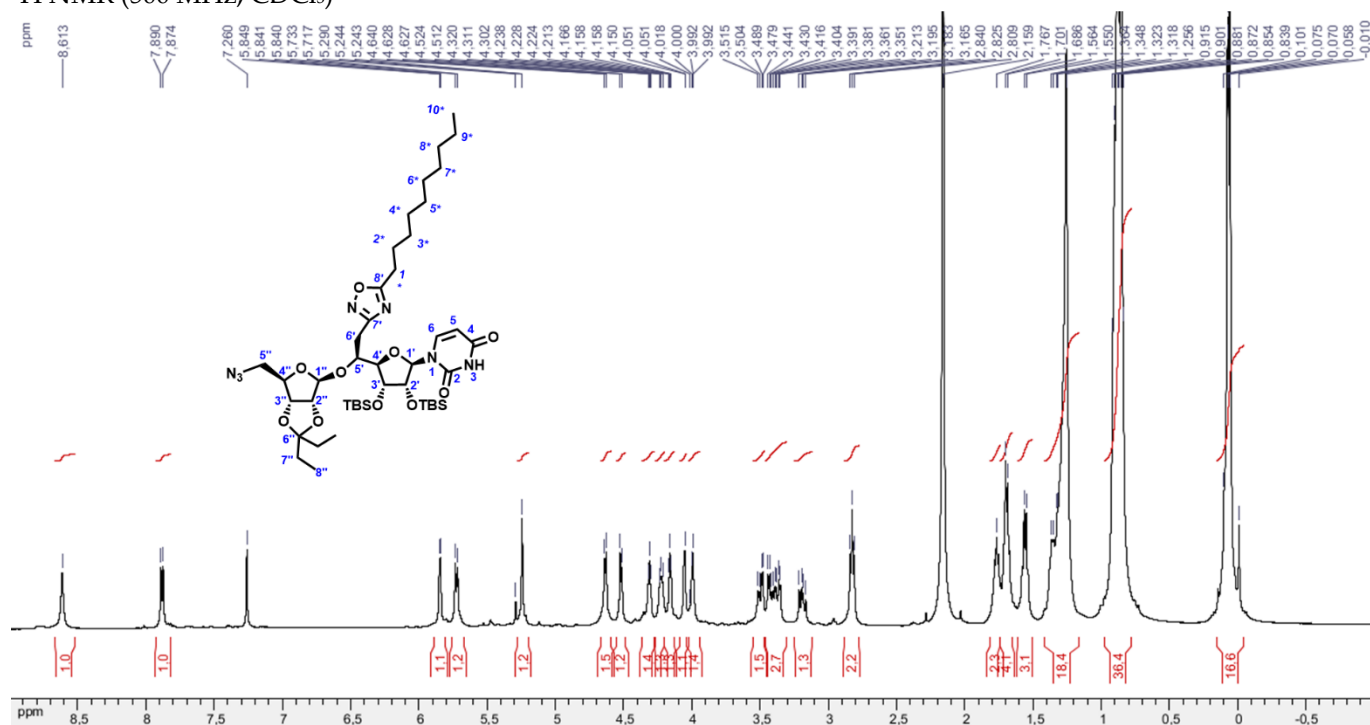


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )

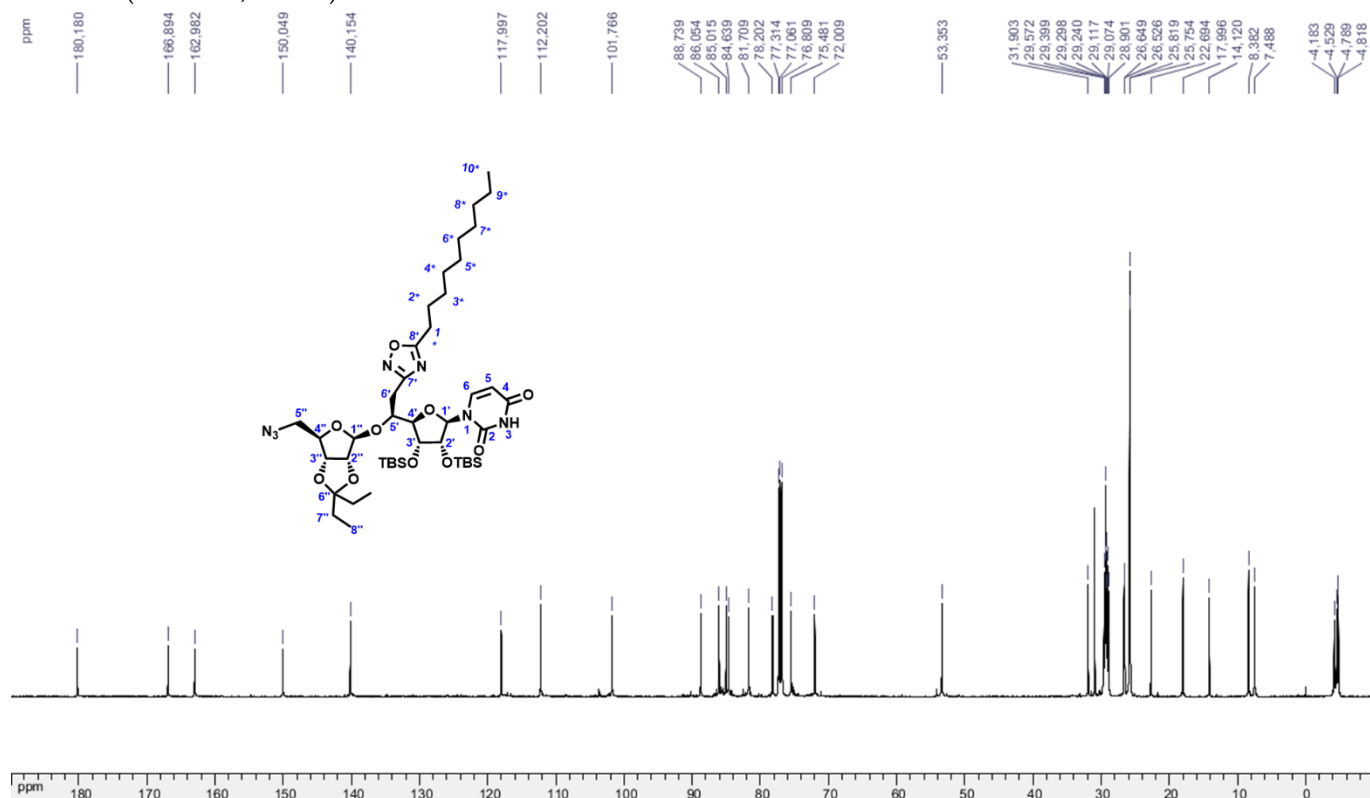


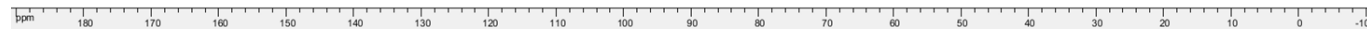
# Protected oxadiazole 11a

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

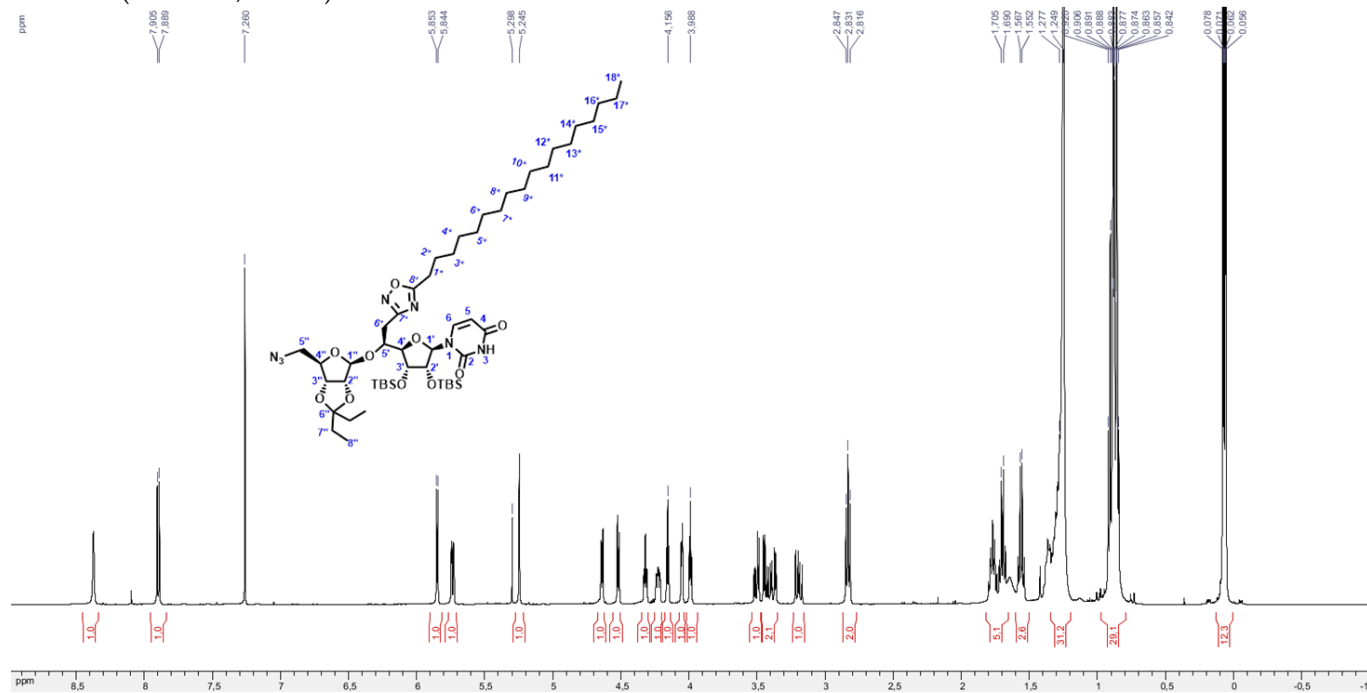
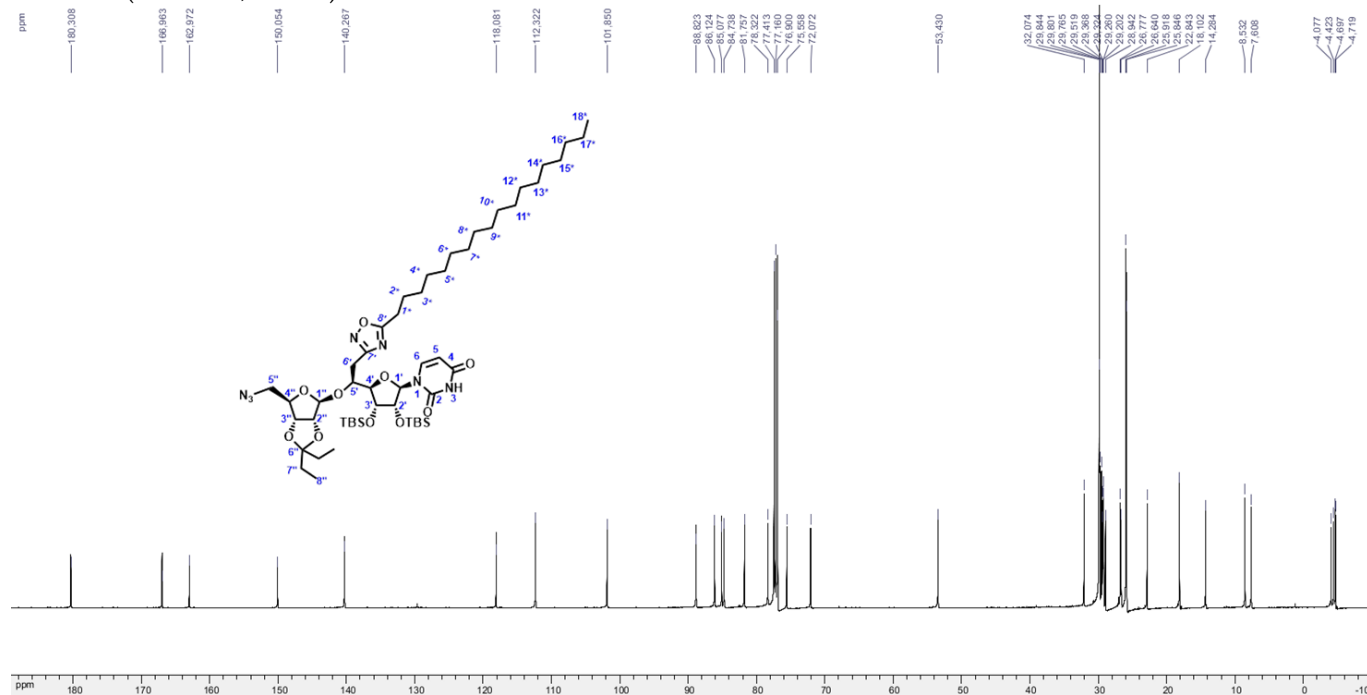


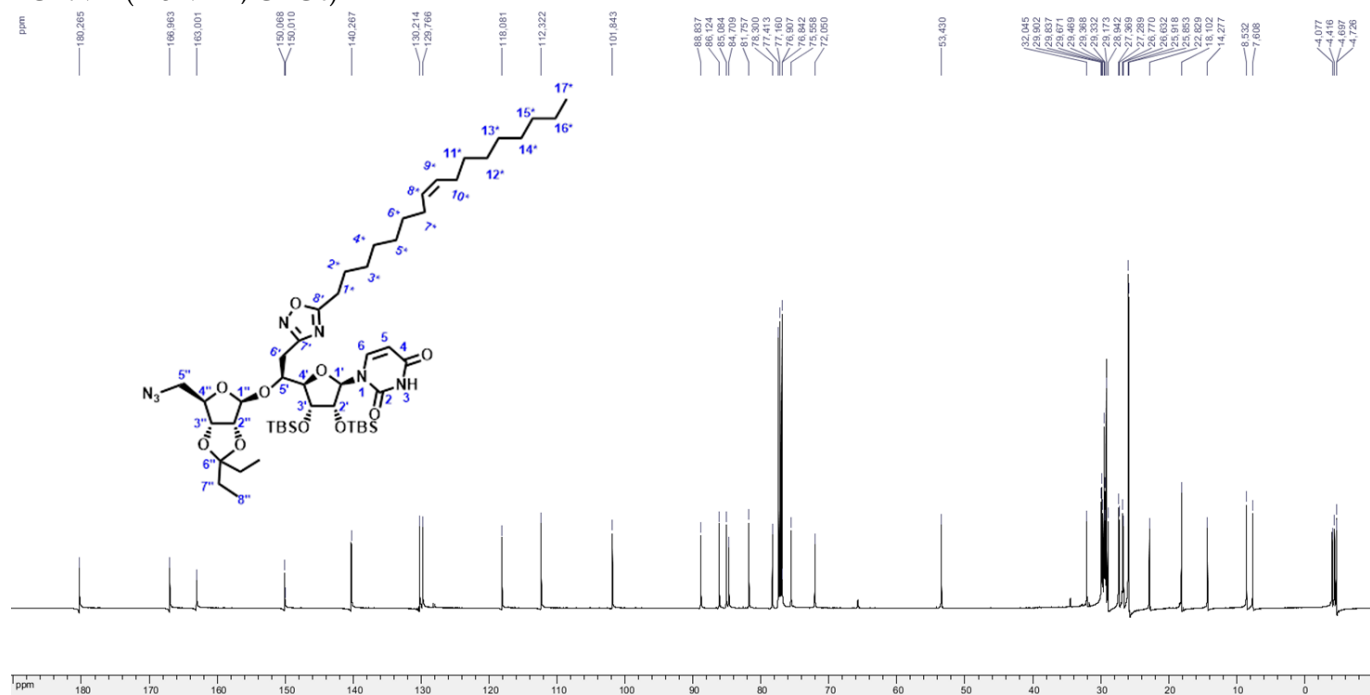
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)

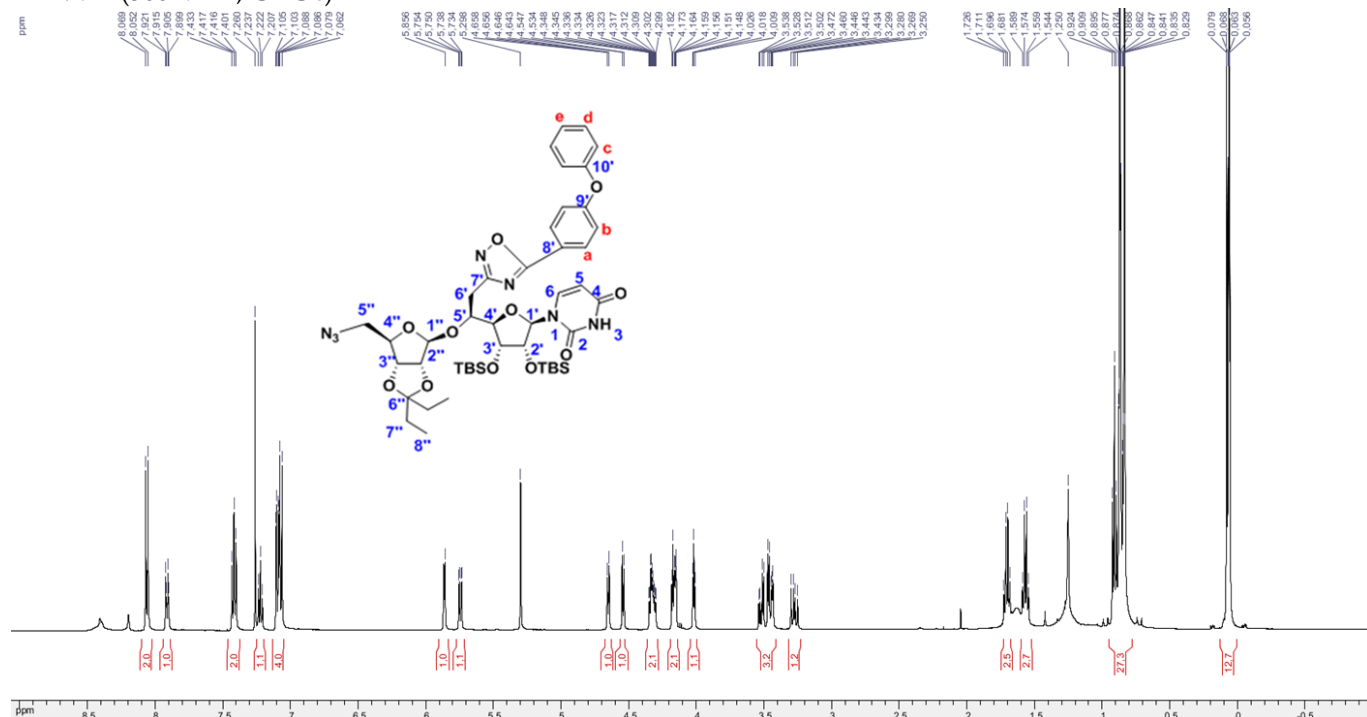


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)

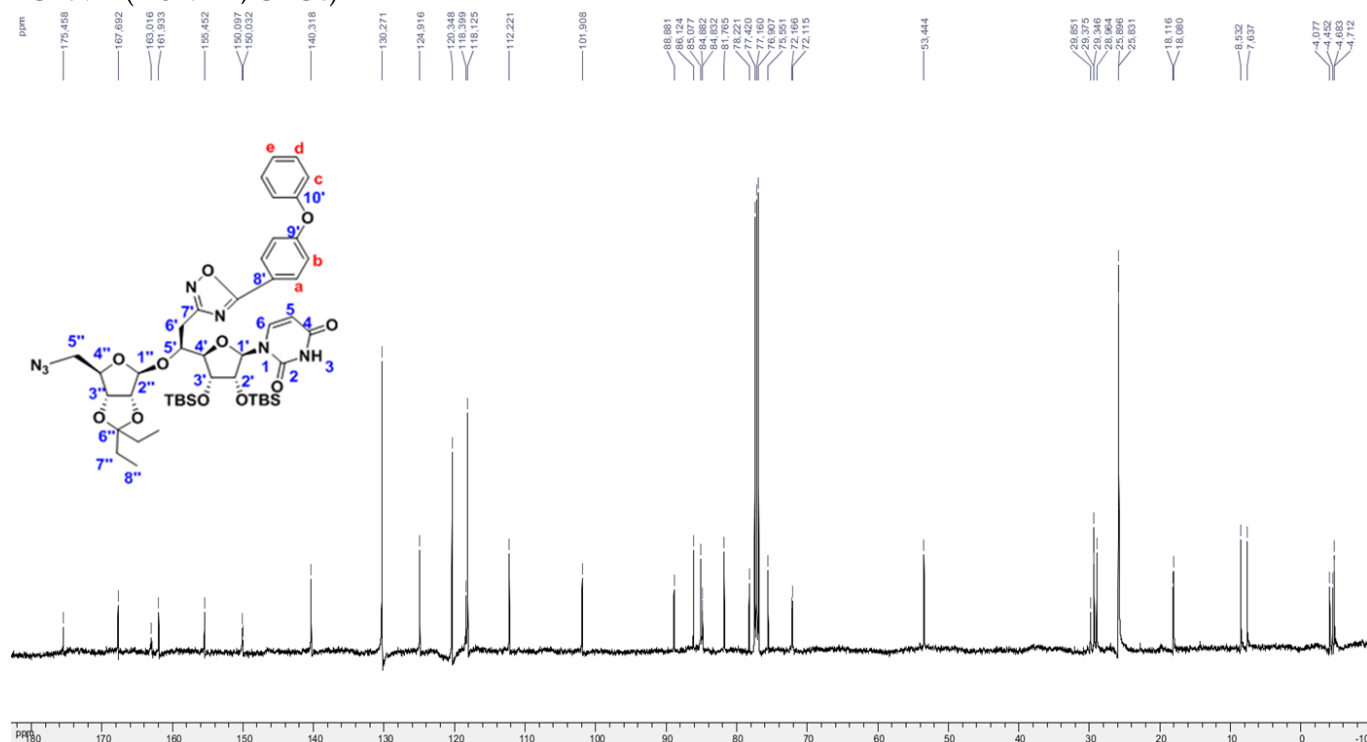
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)

# Protected Oxadiazole 11e

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)

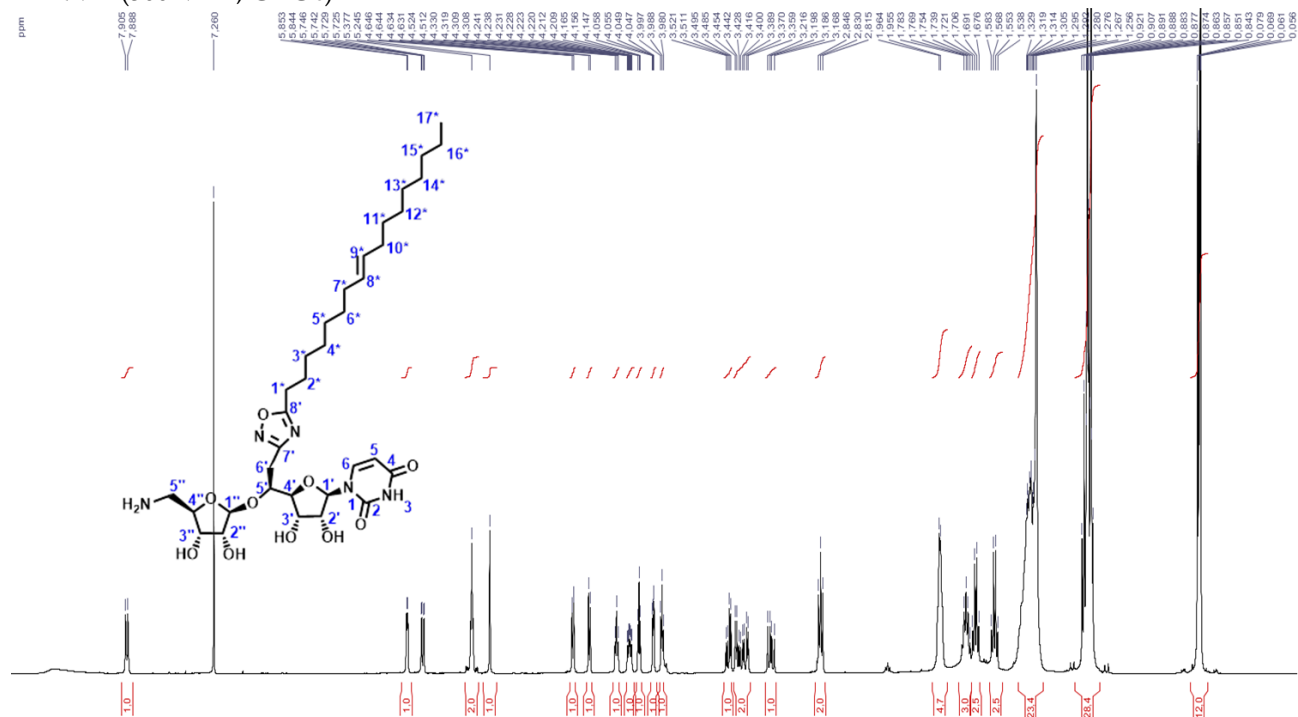


<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)

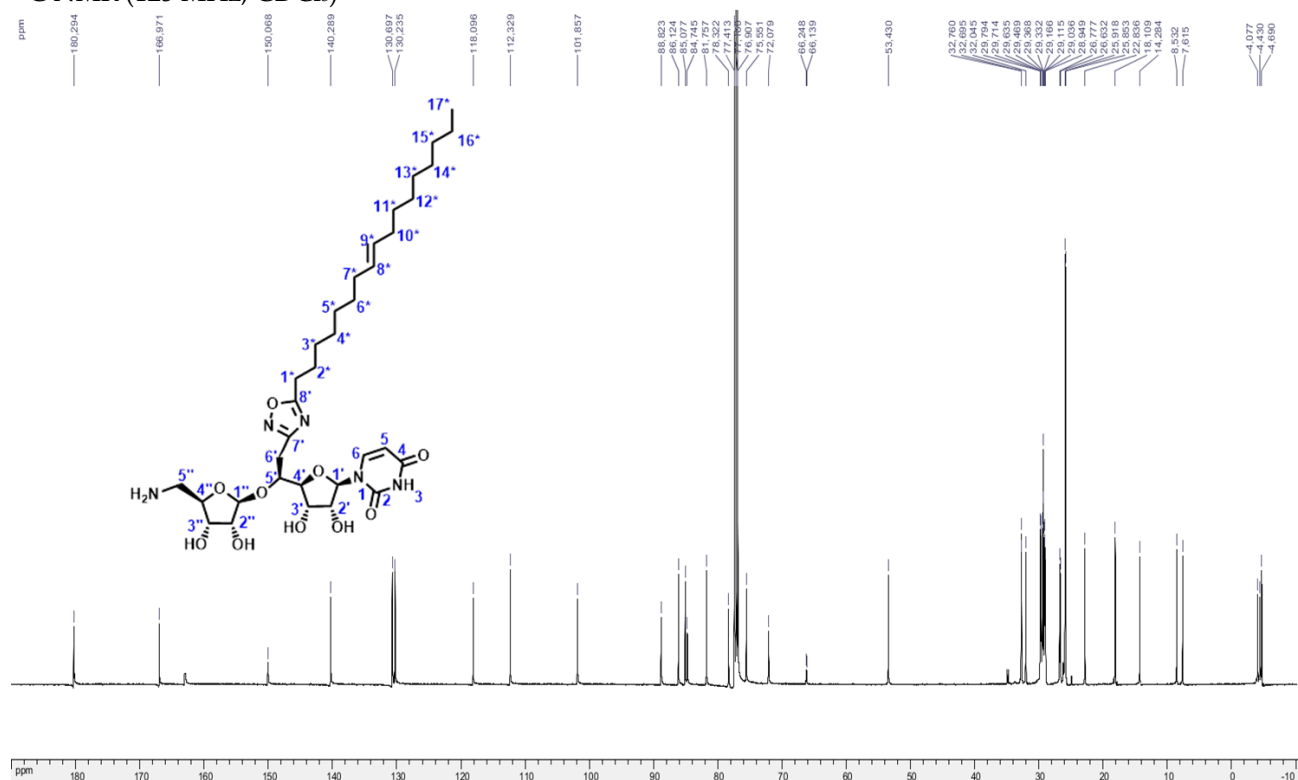


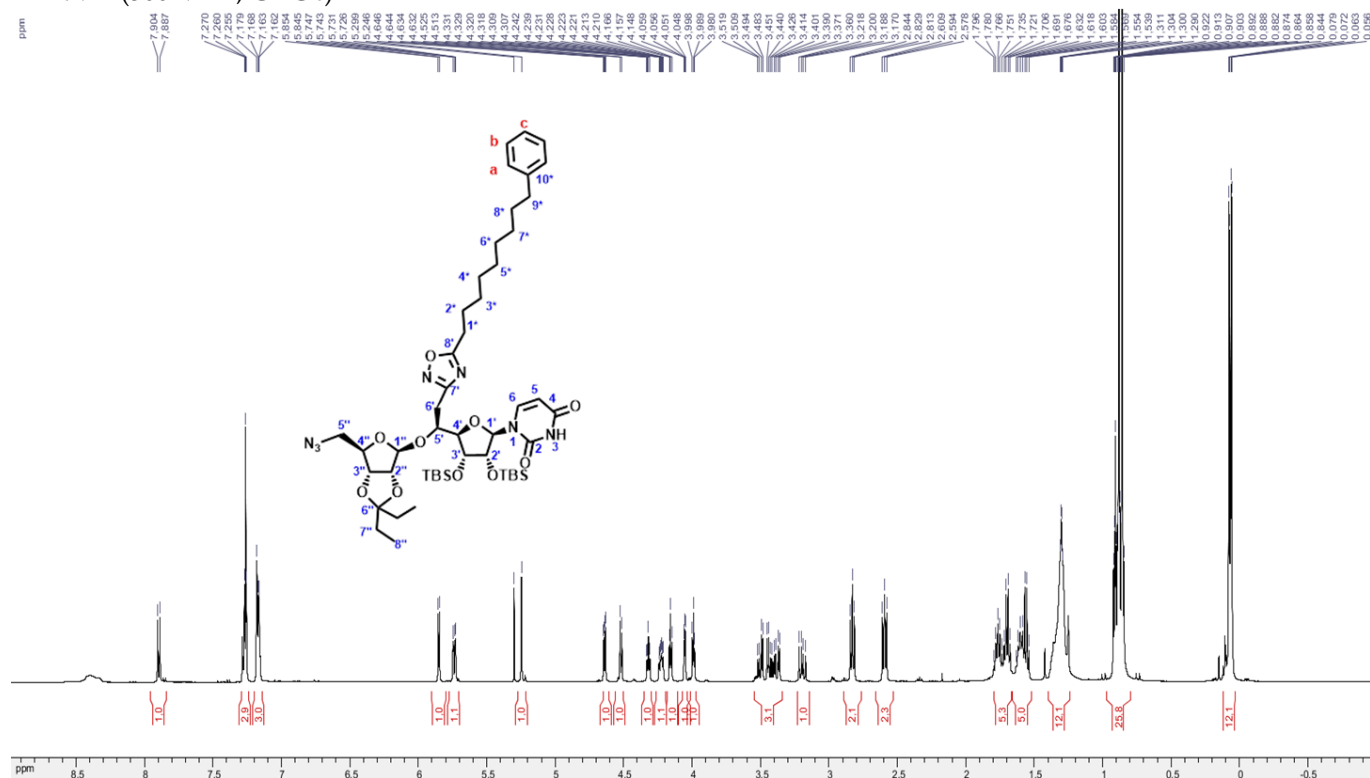
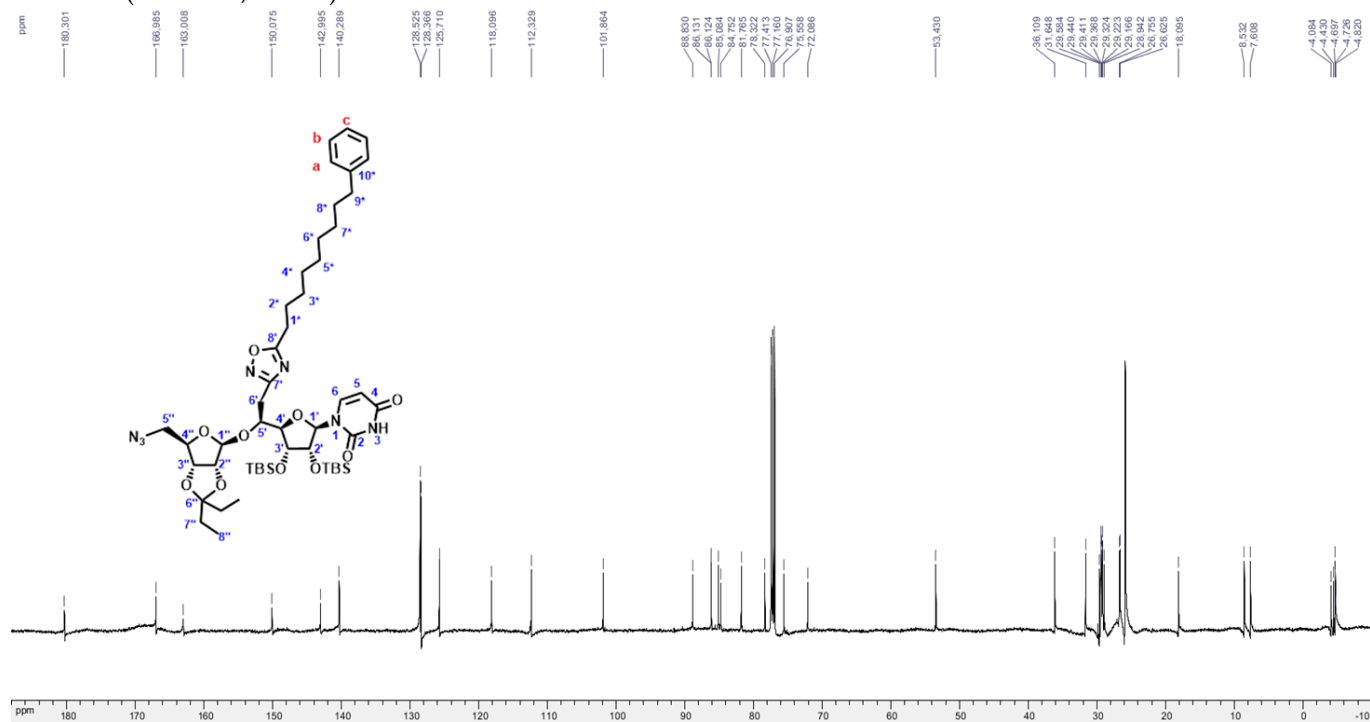
# Protected Oxadiazole 11f

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



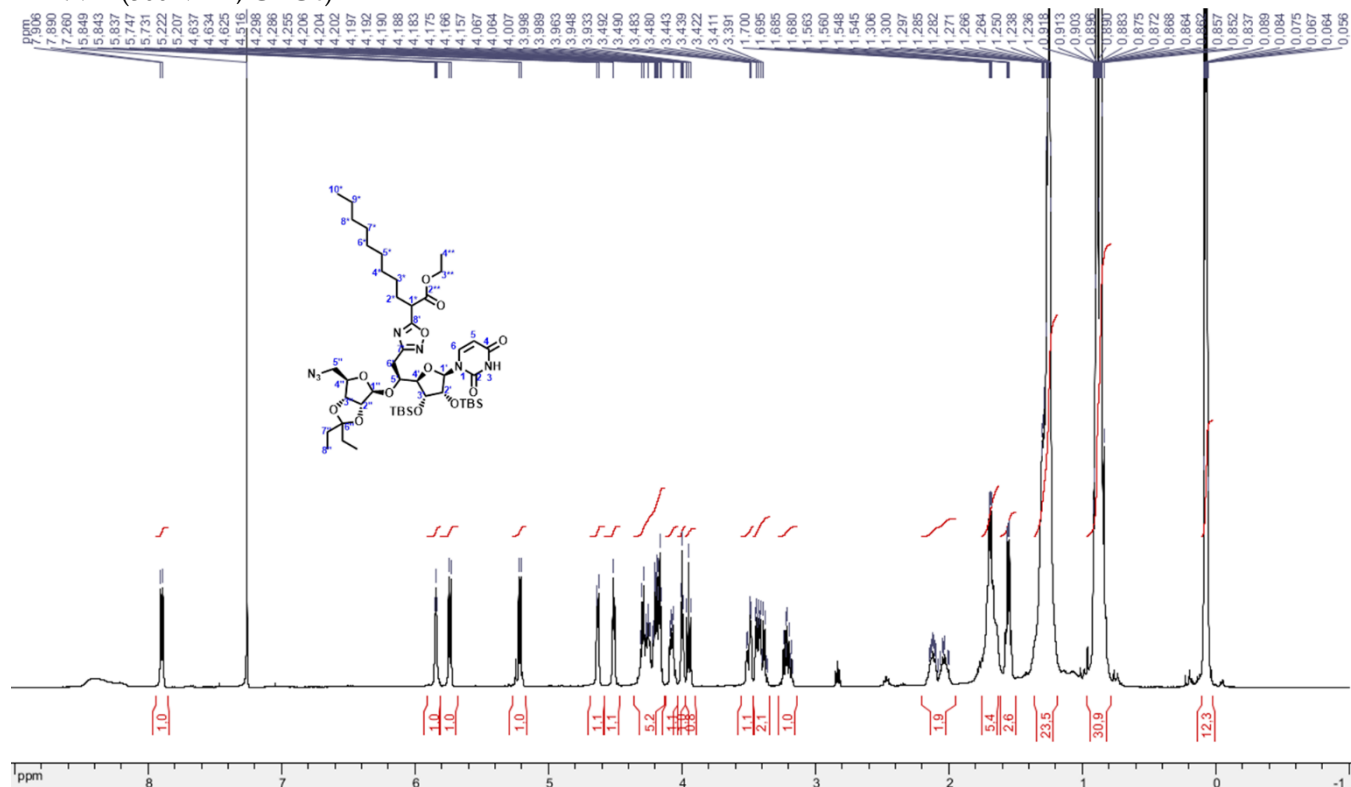
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



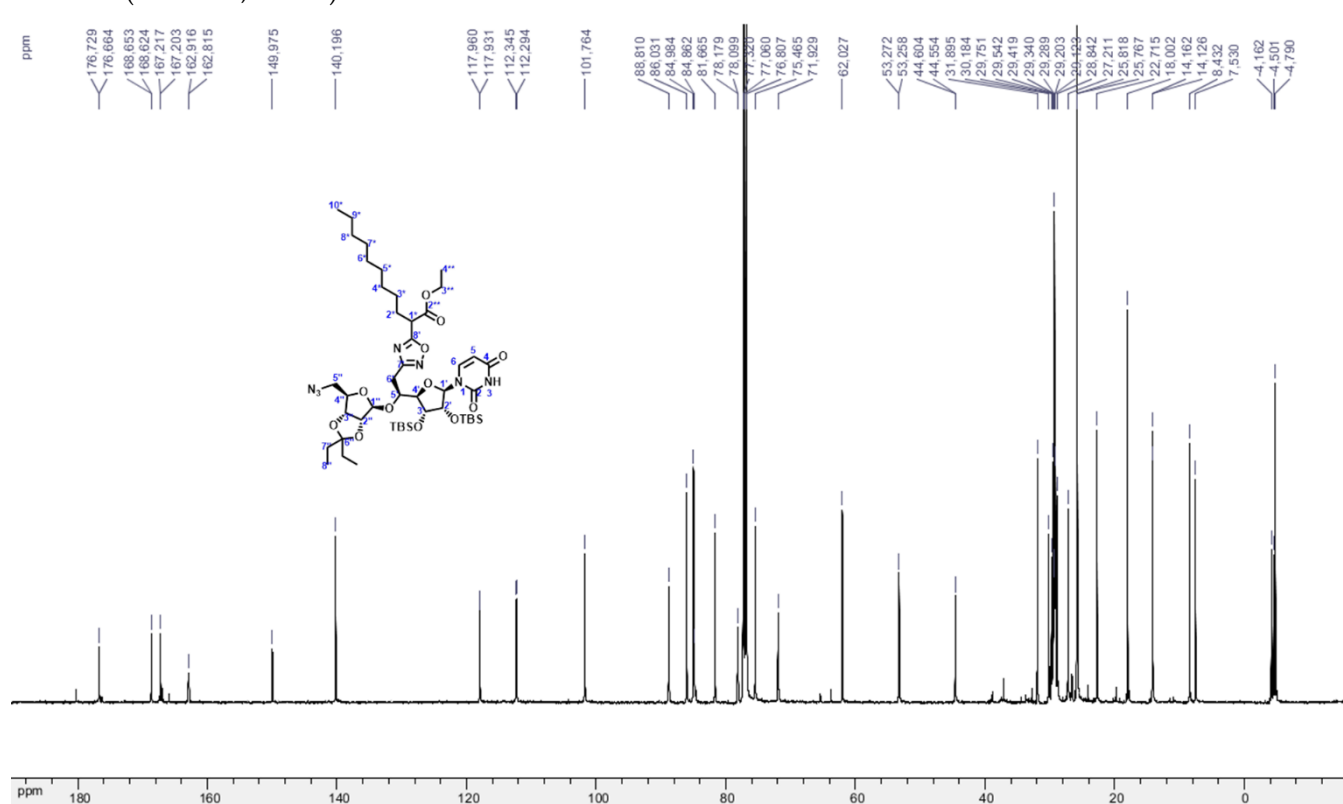
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)

# Protected Oxadiazole 11h

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)

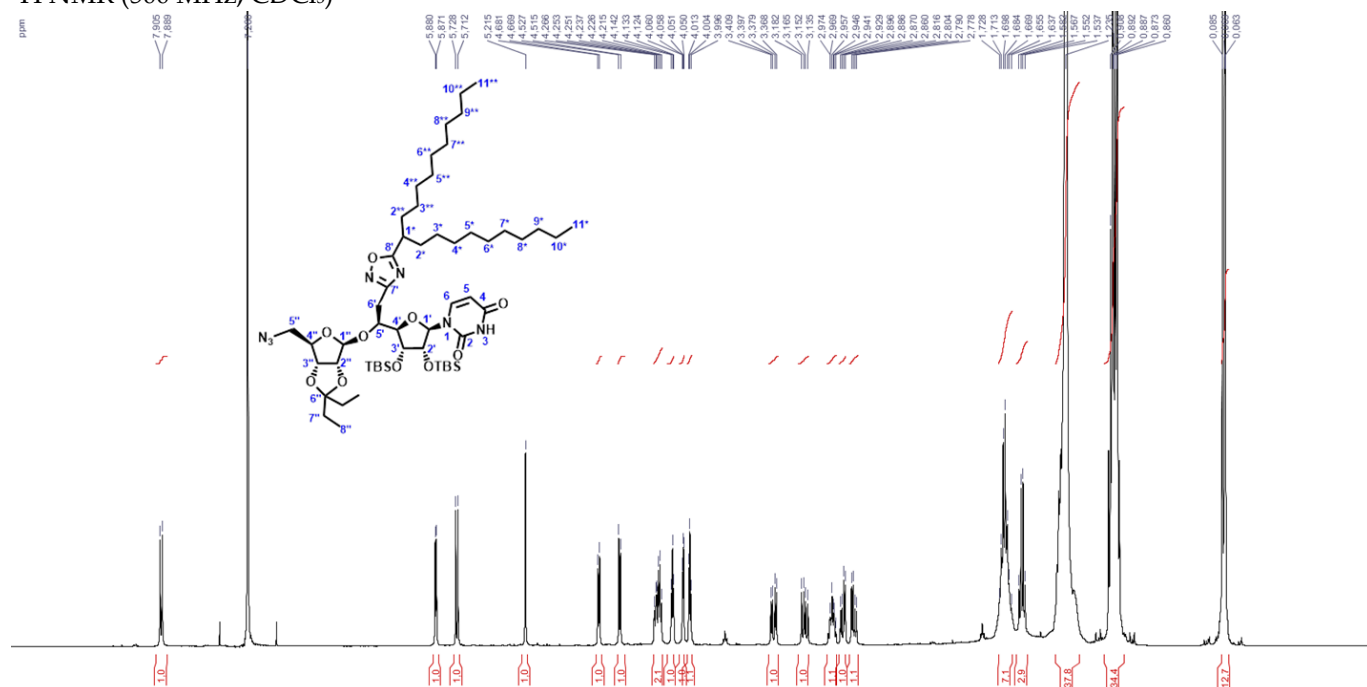


<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)

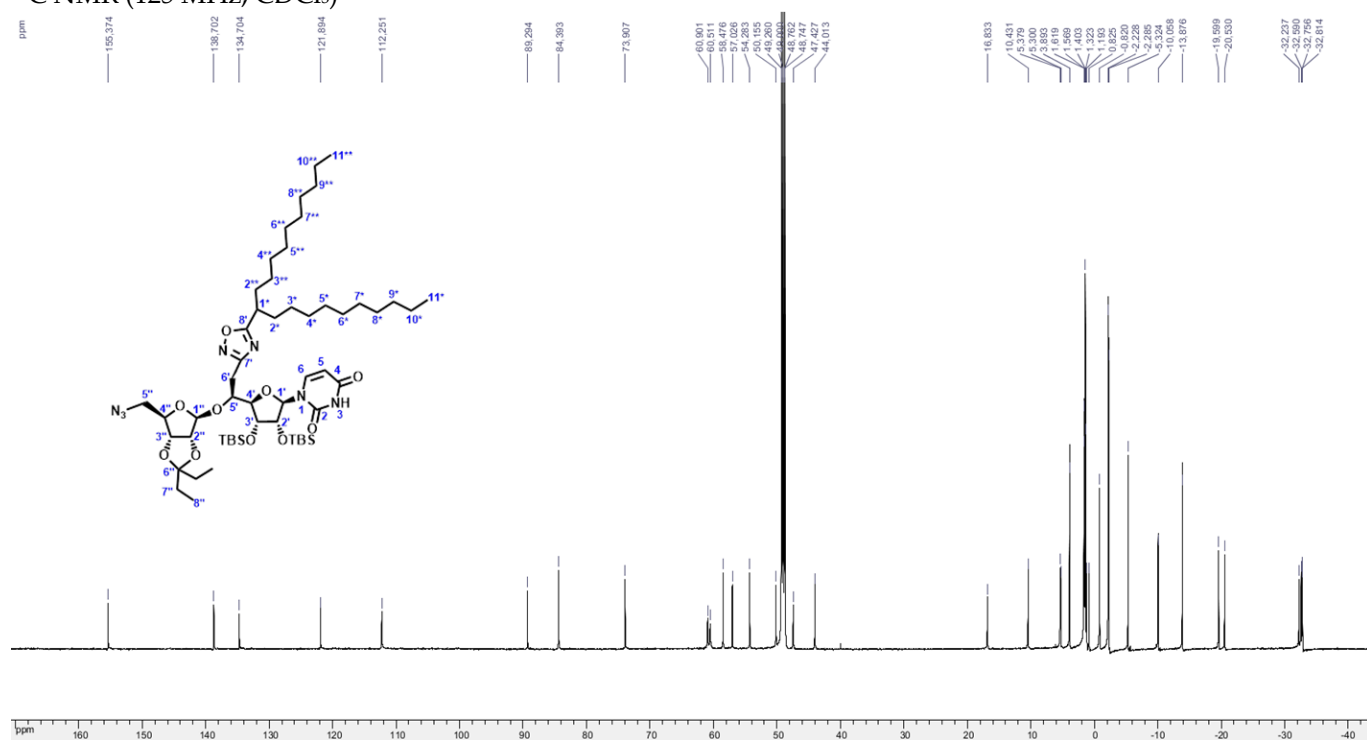


# Protected Oxadiazole 11i

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)

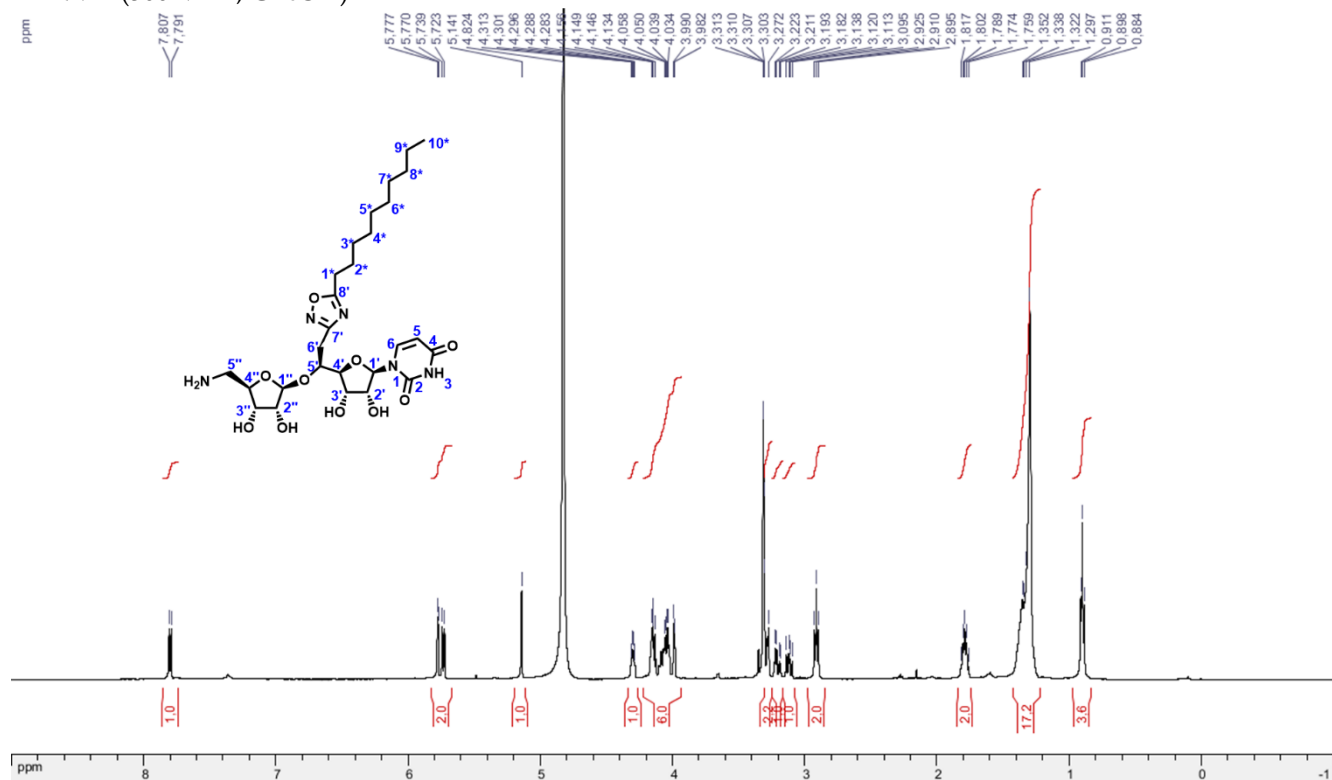


<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)

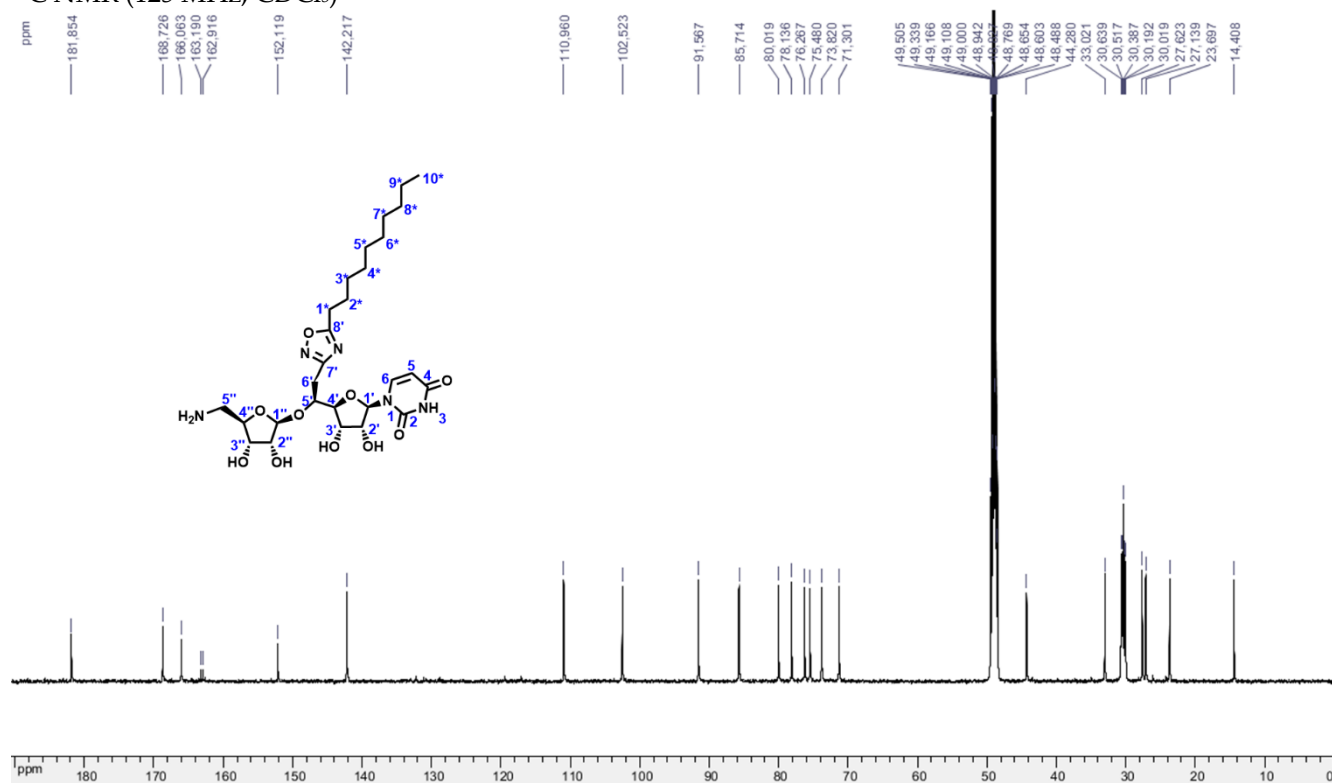


# **Oxadiazole 12a**

$^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ )



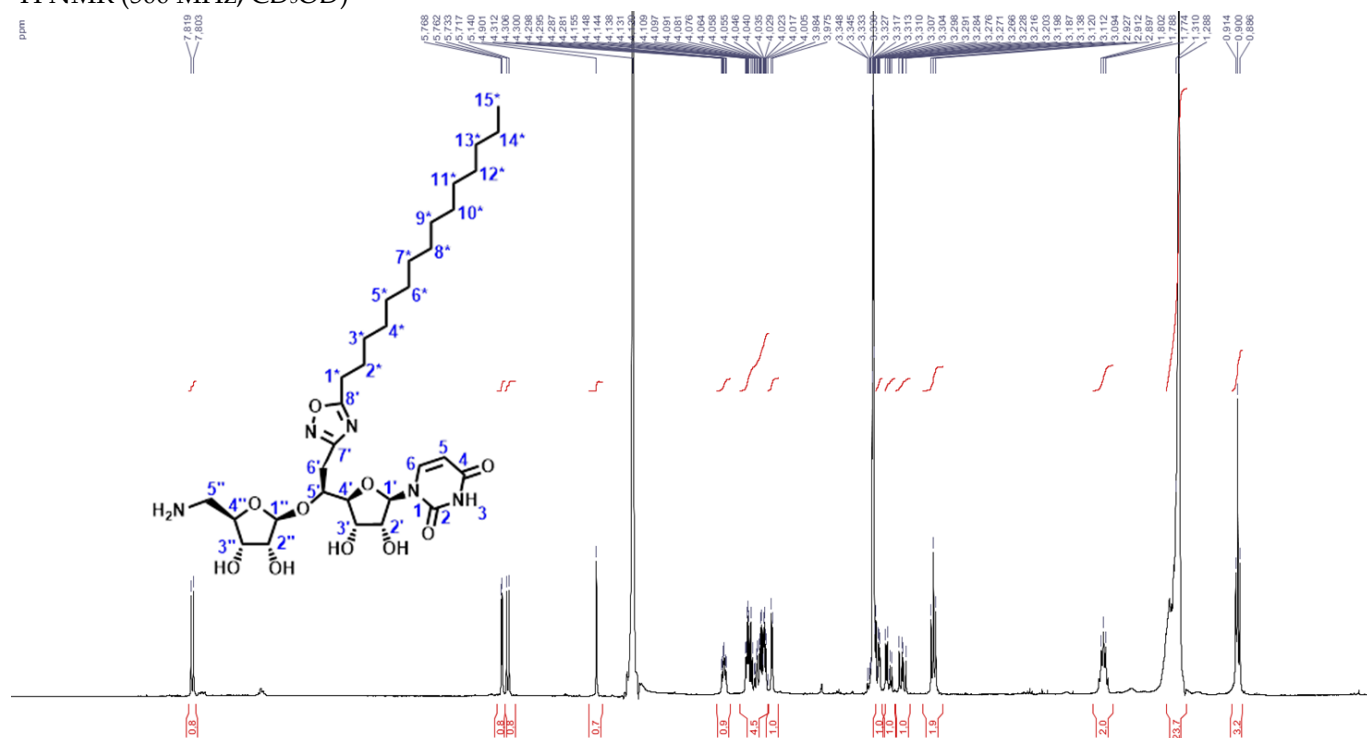
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



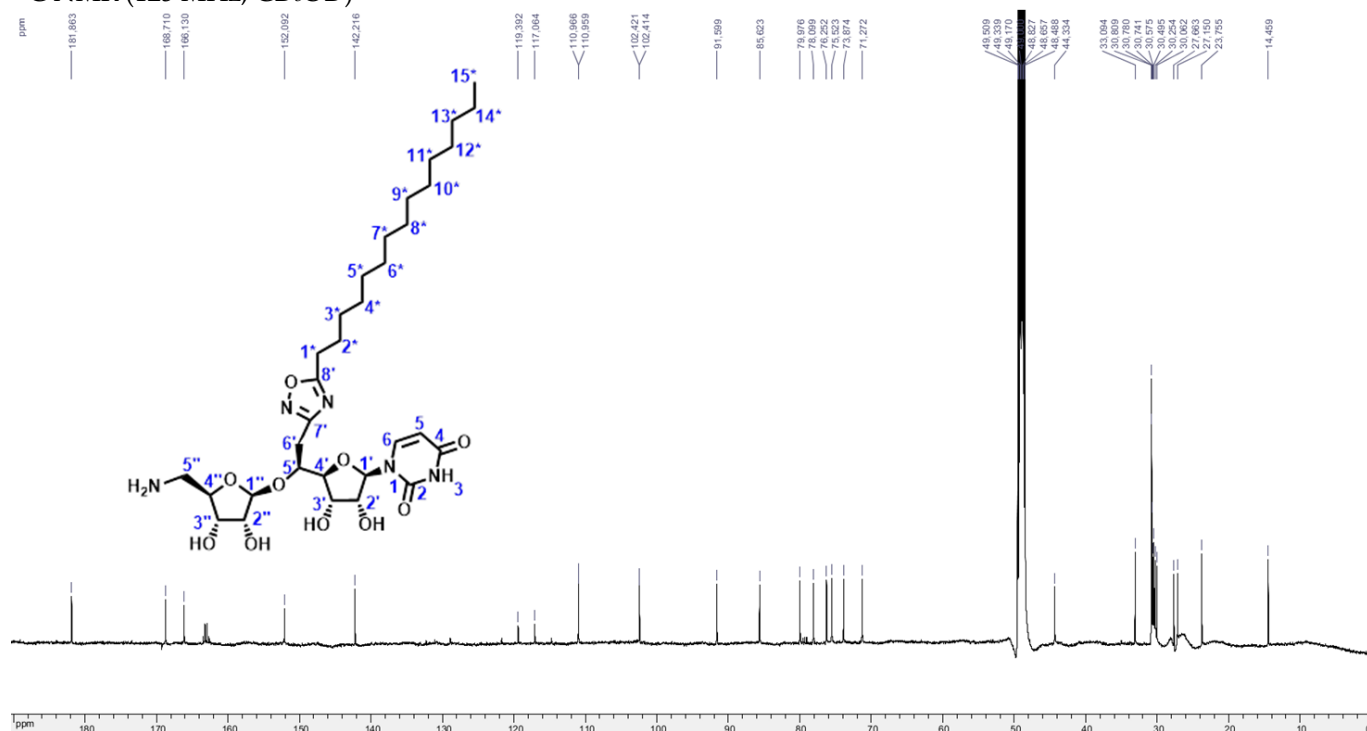


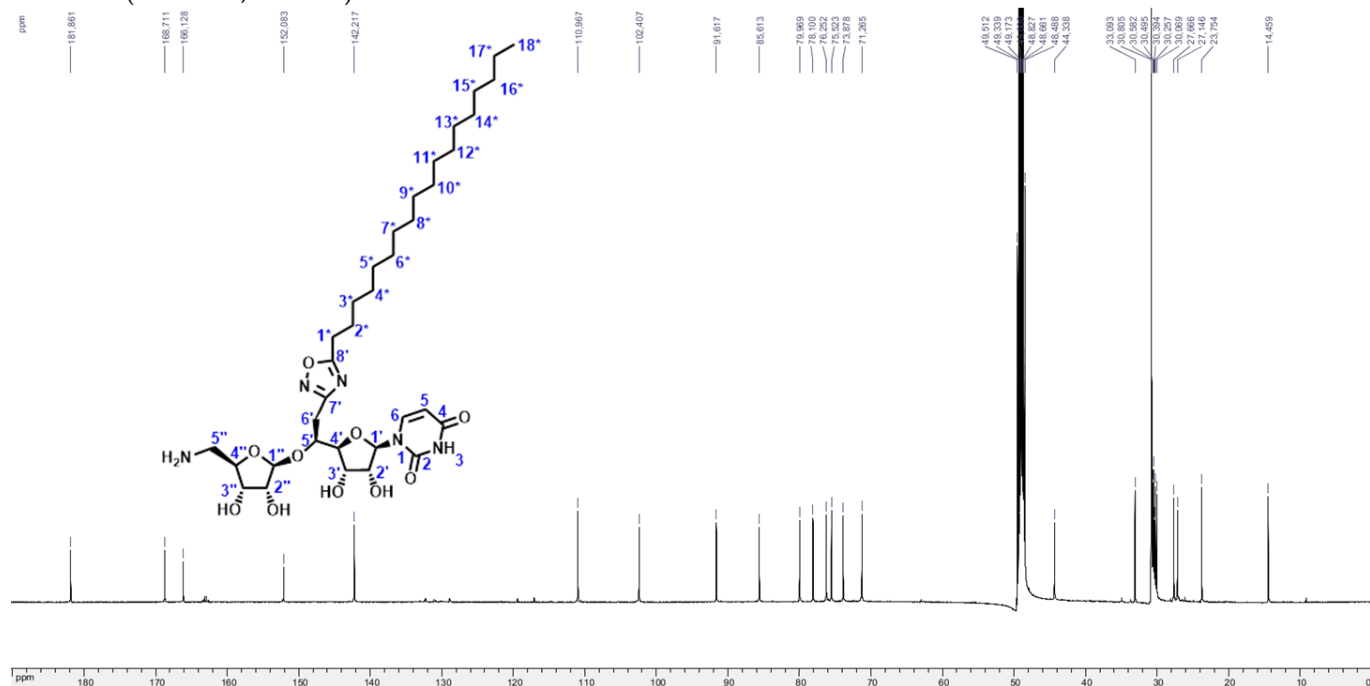
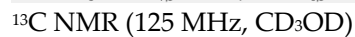
# **Oxadiazole 12b**

$^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ )



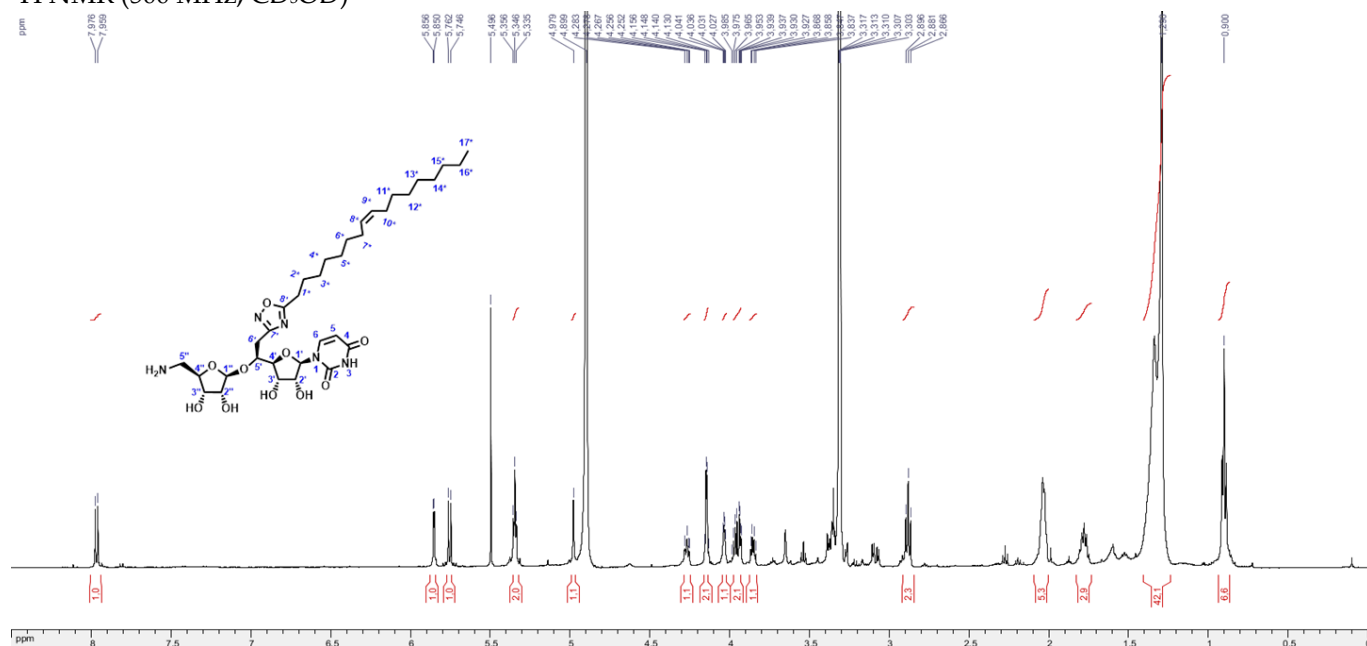
$^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ )



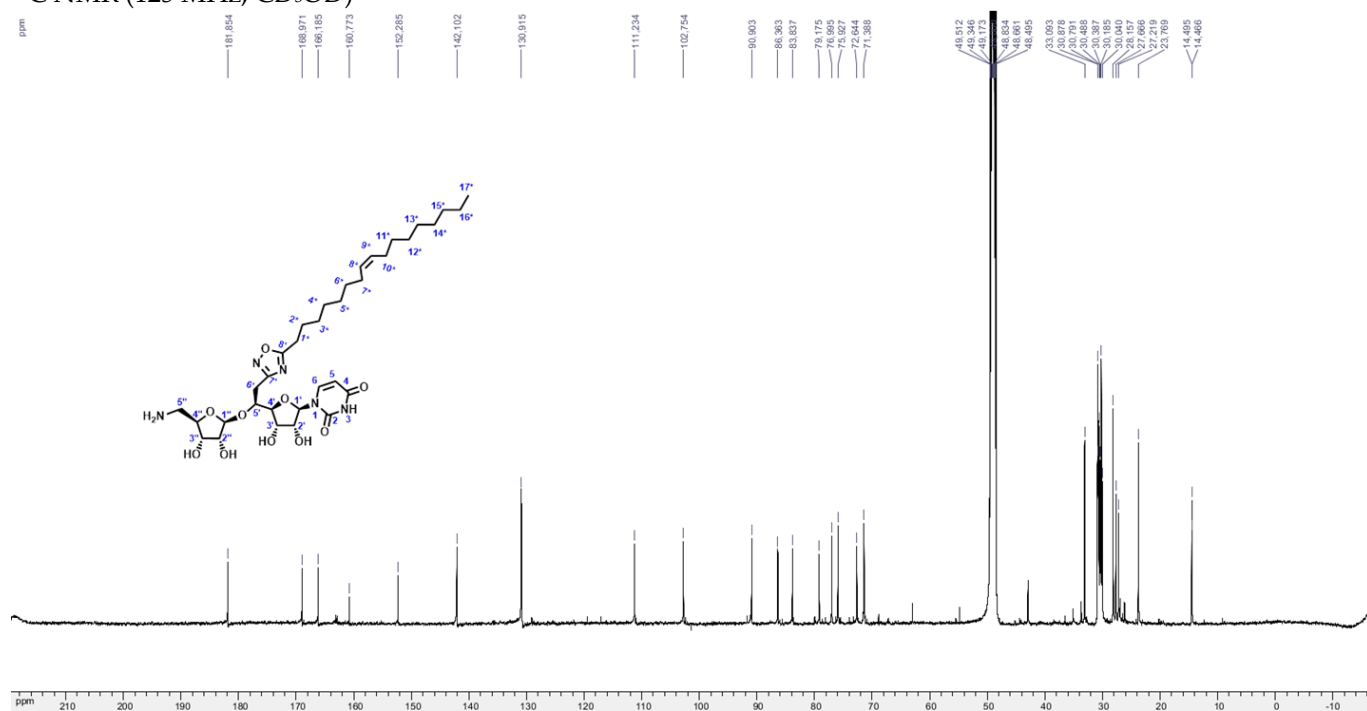
<sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)

# Oxadiazole 12d

$^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ )

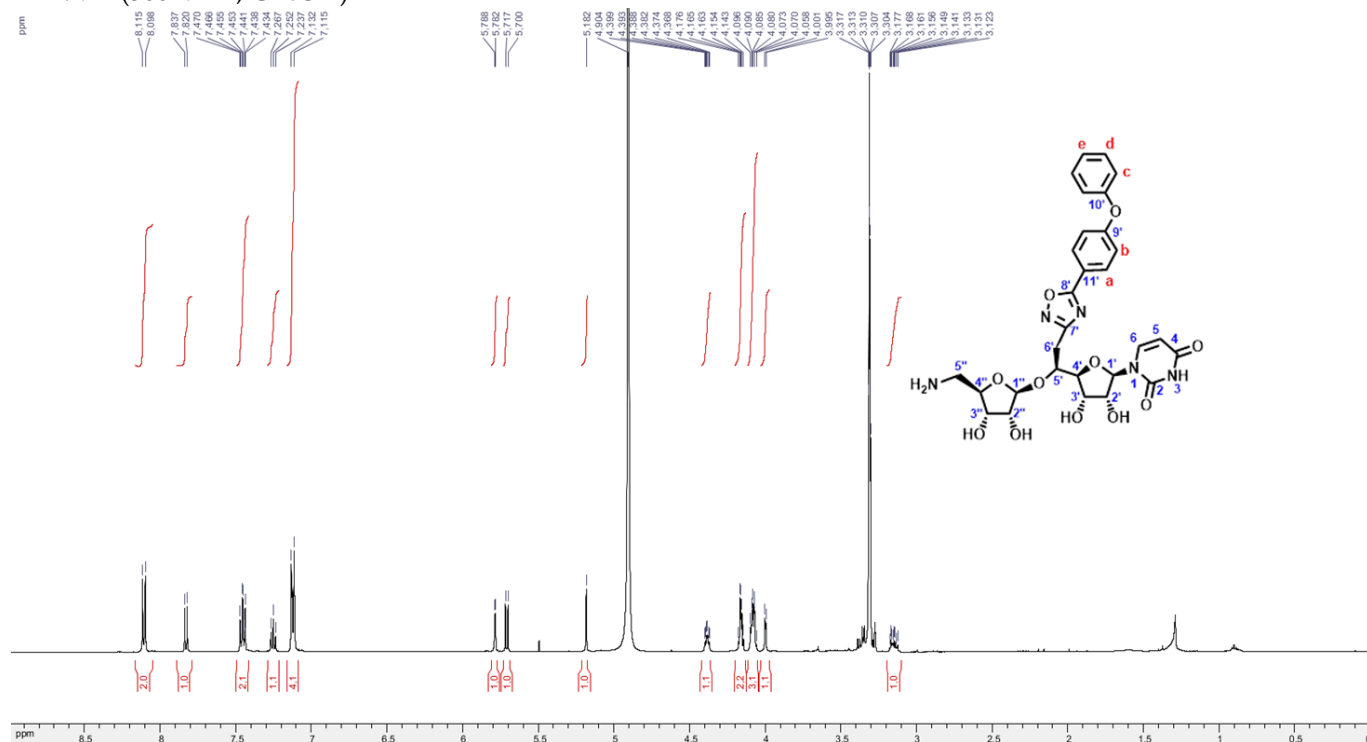


$^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ )

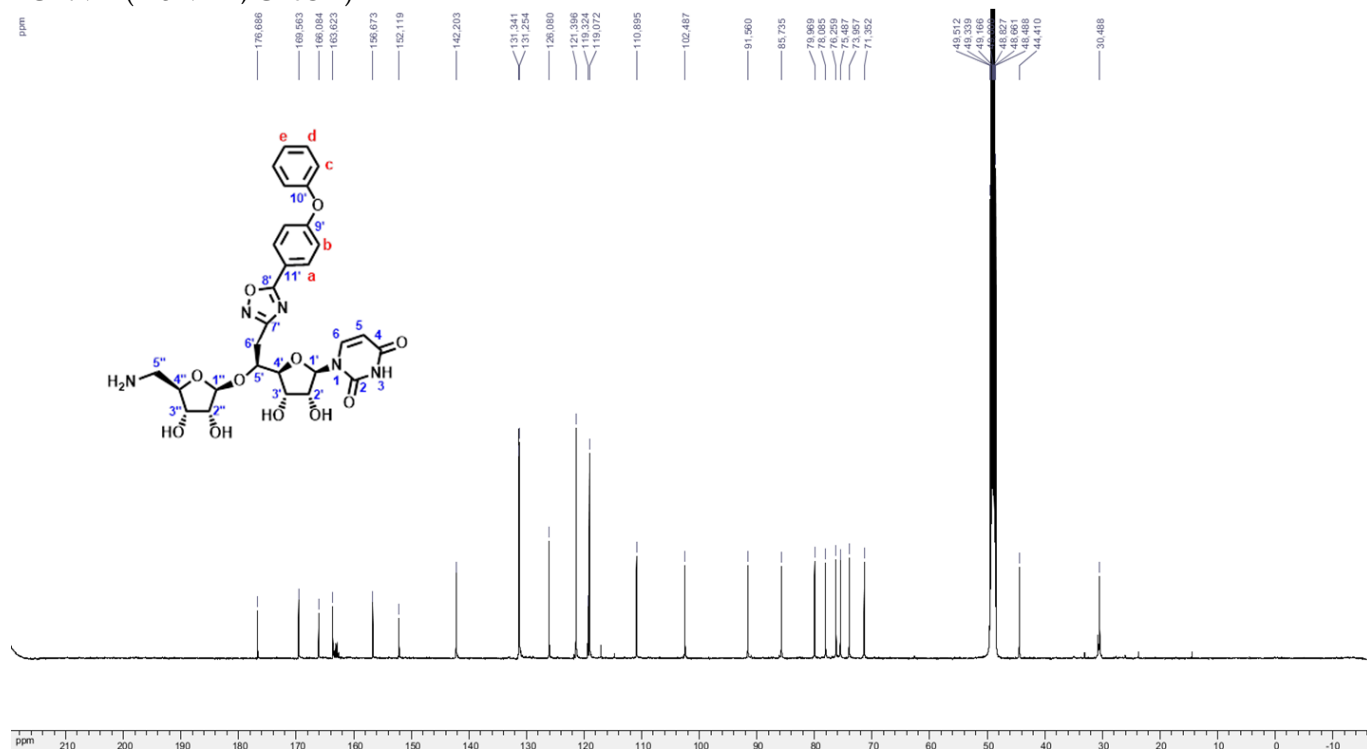


# **Oxadiazole 12e**

<sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)

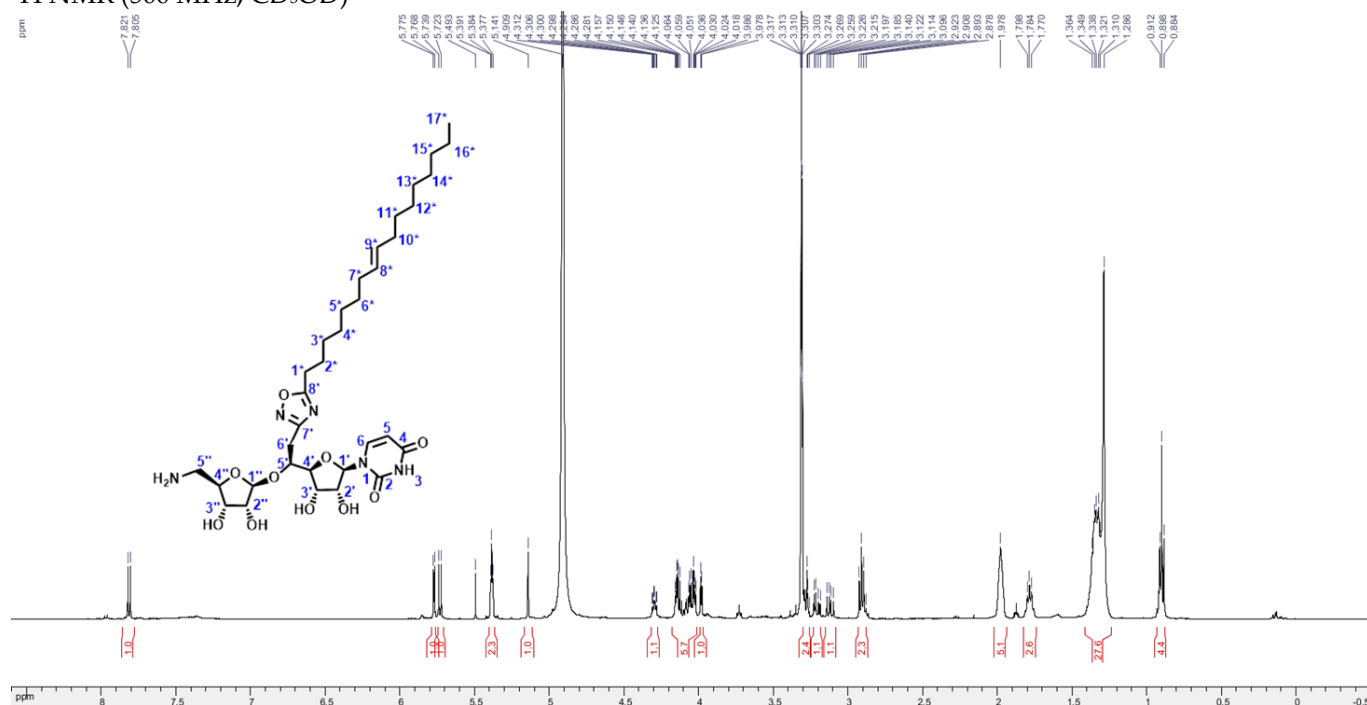


<sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)

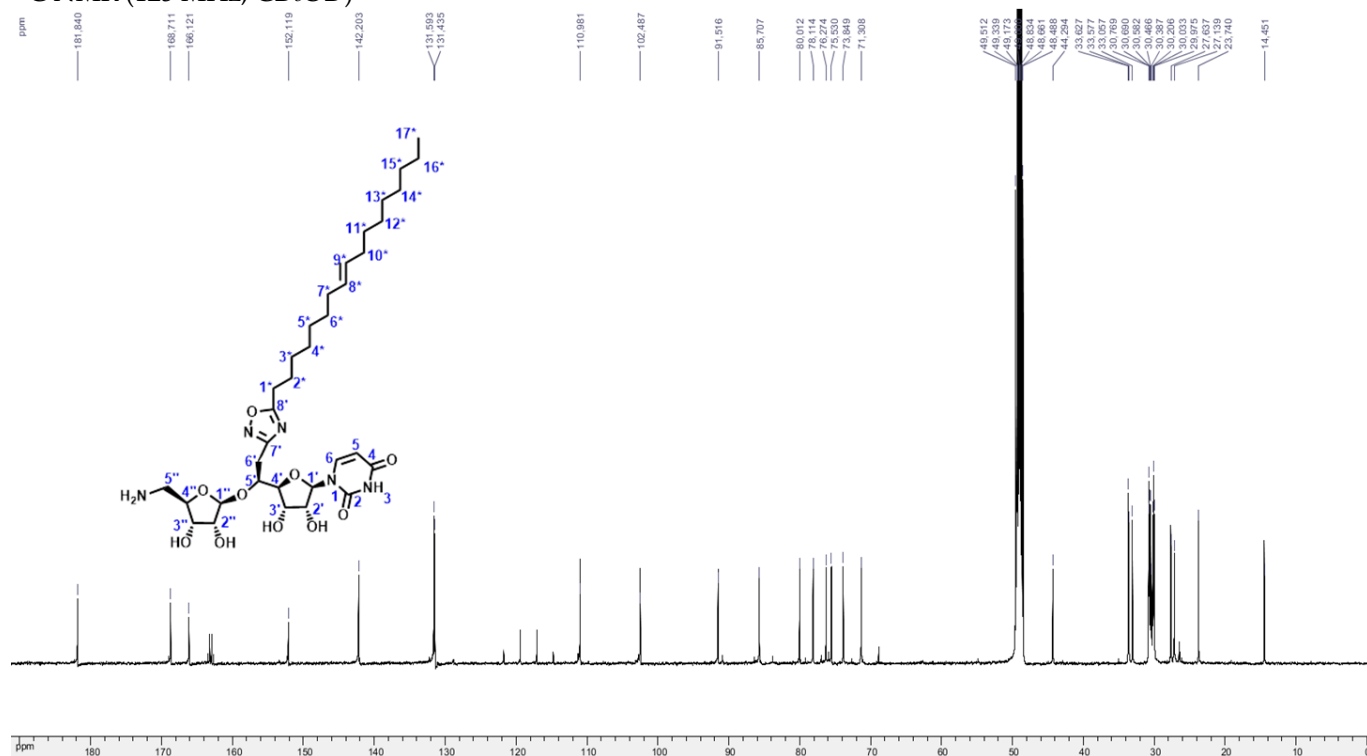


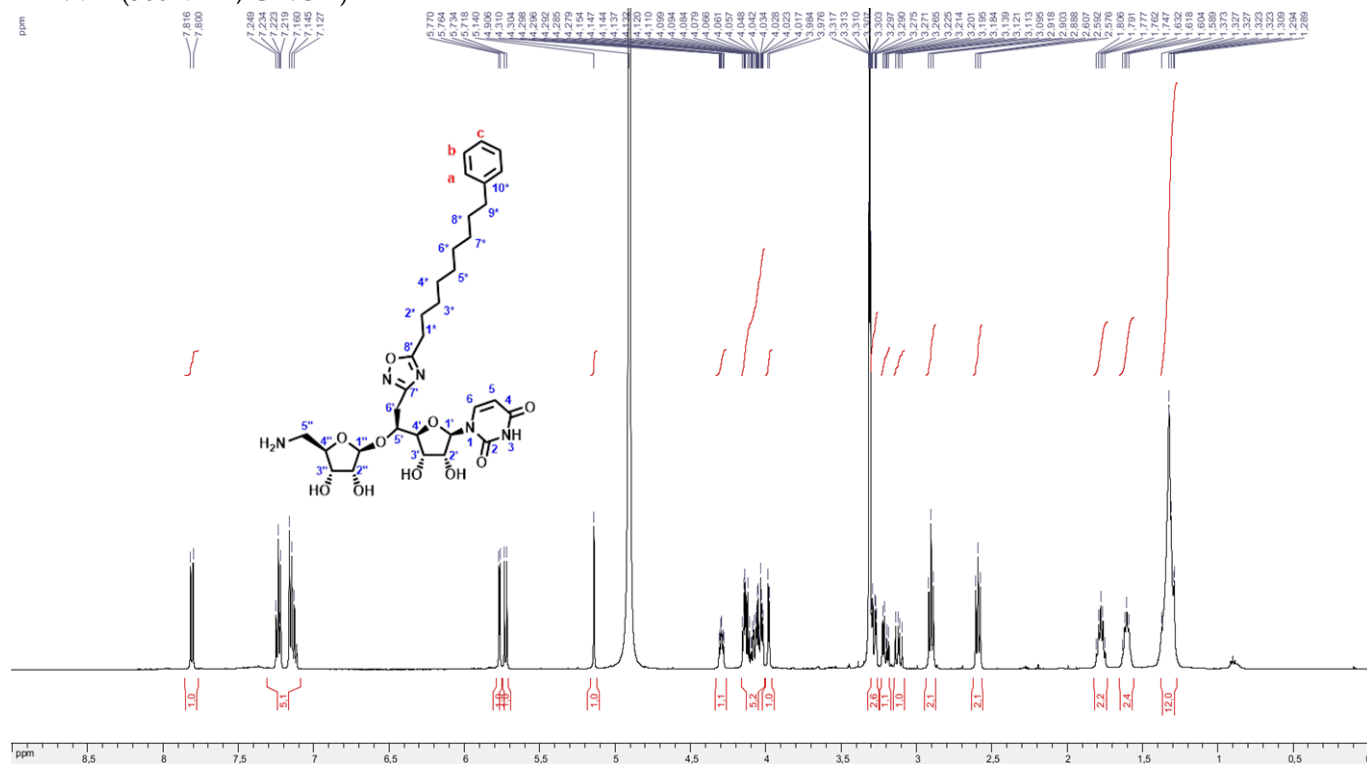
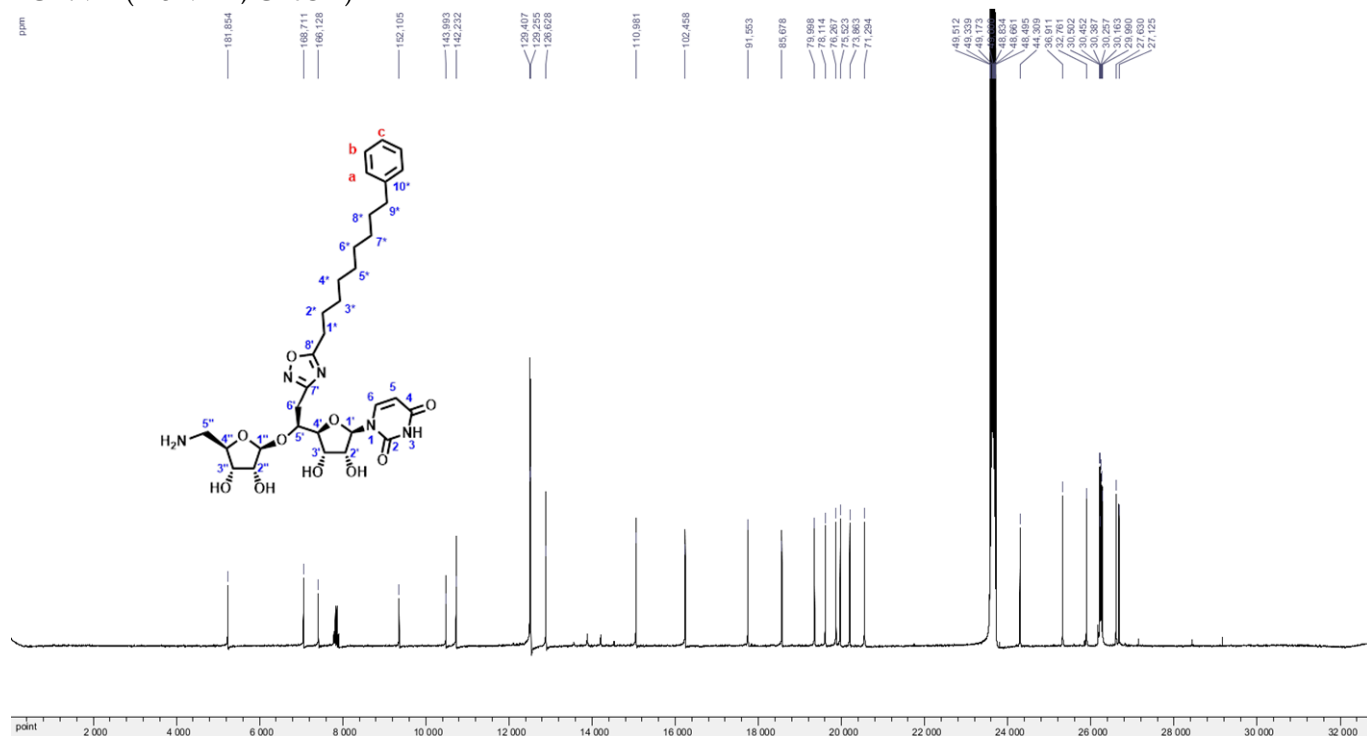
# Oxadiazole 12f

<sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)



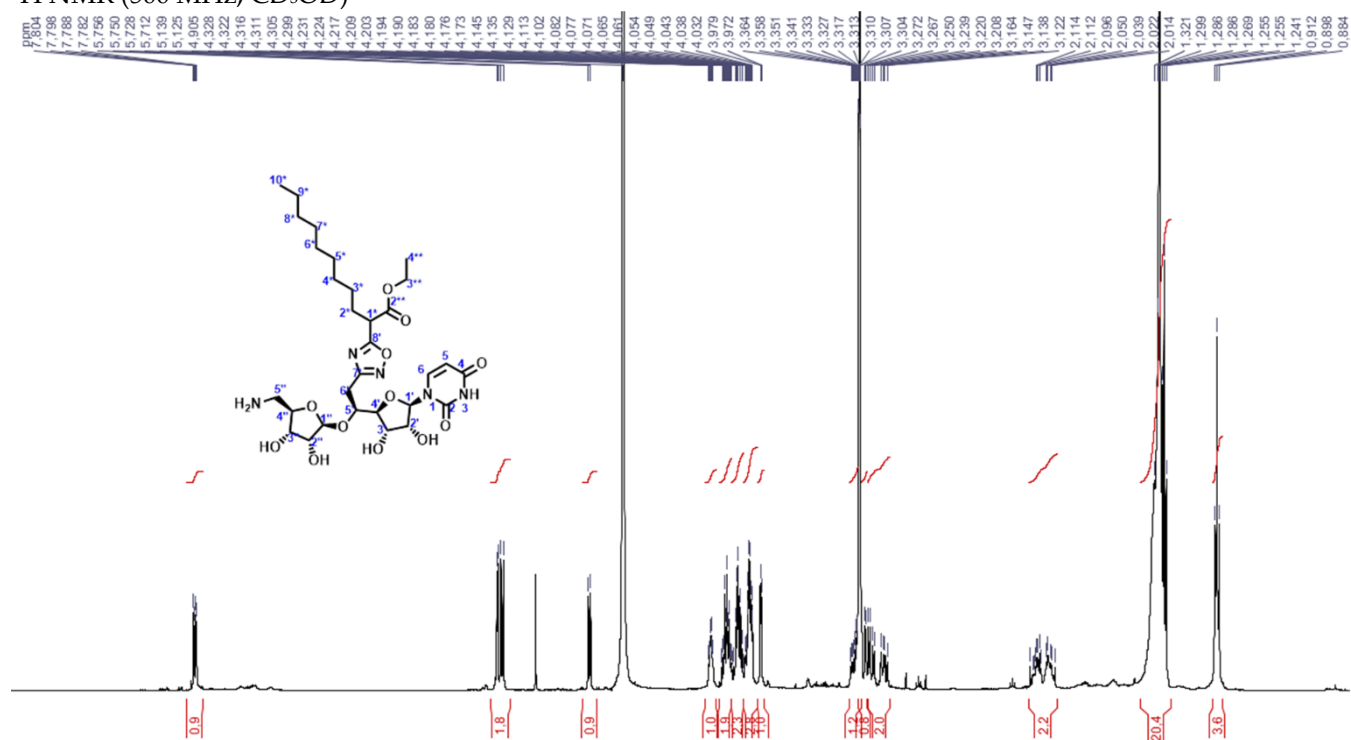
<sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)



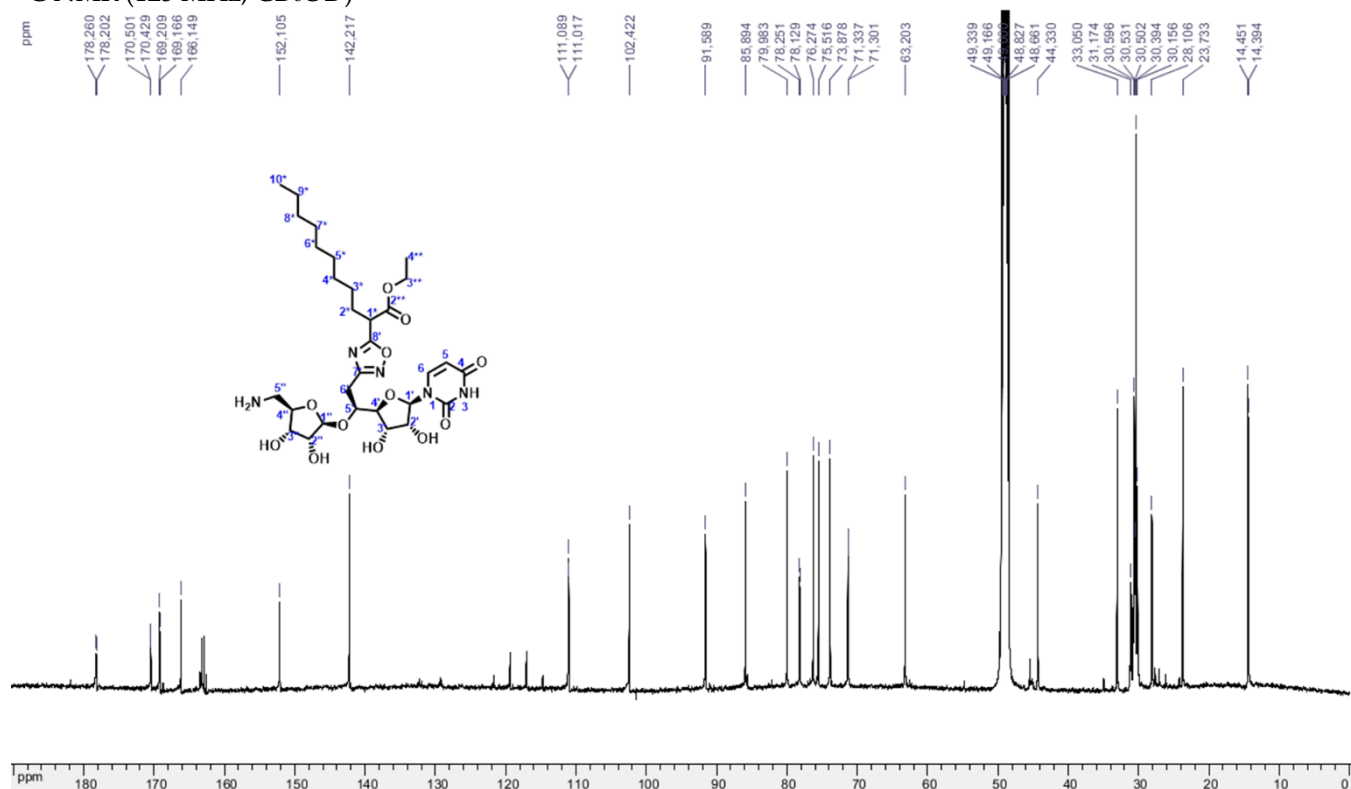
<sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)<sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)<sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)

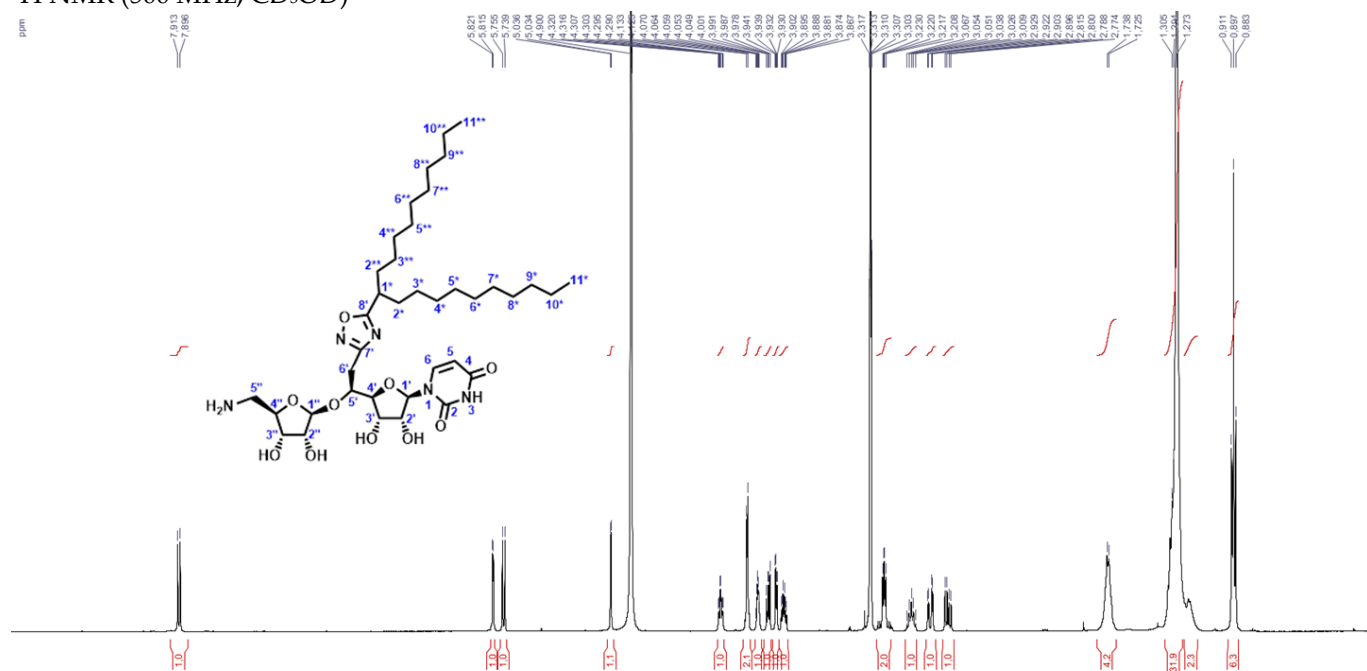
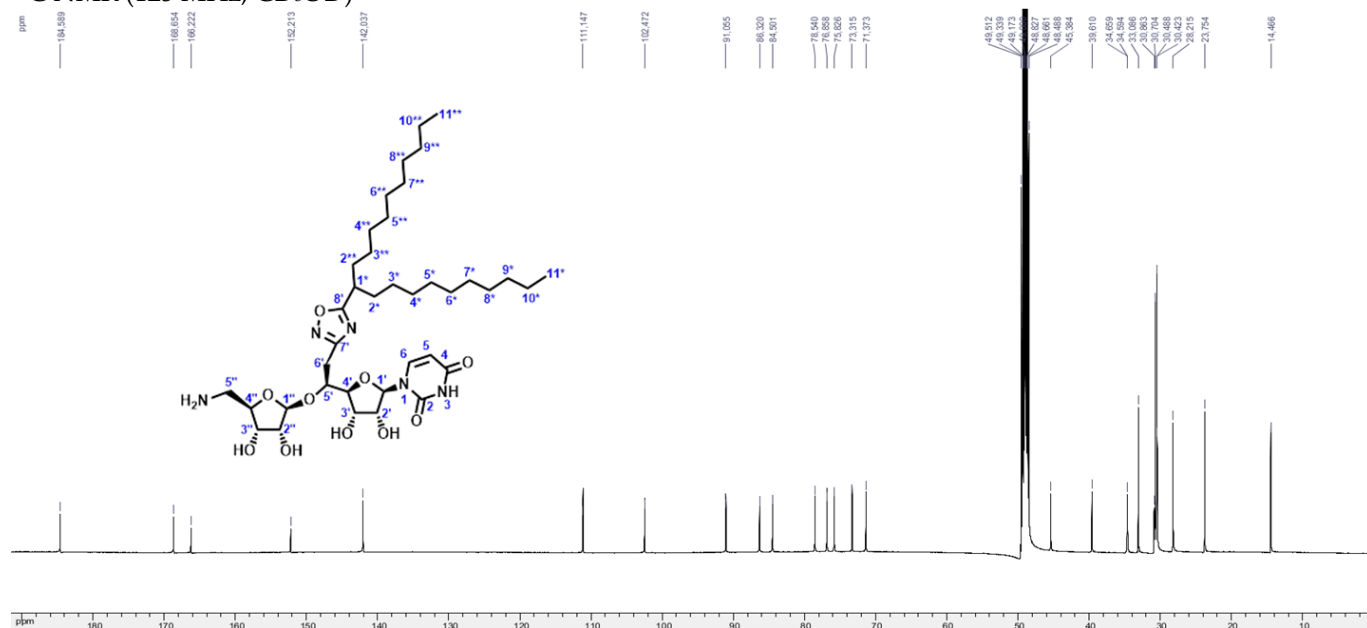
# **Oxadiazole 12h**

<sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)



<sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)

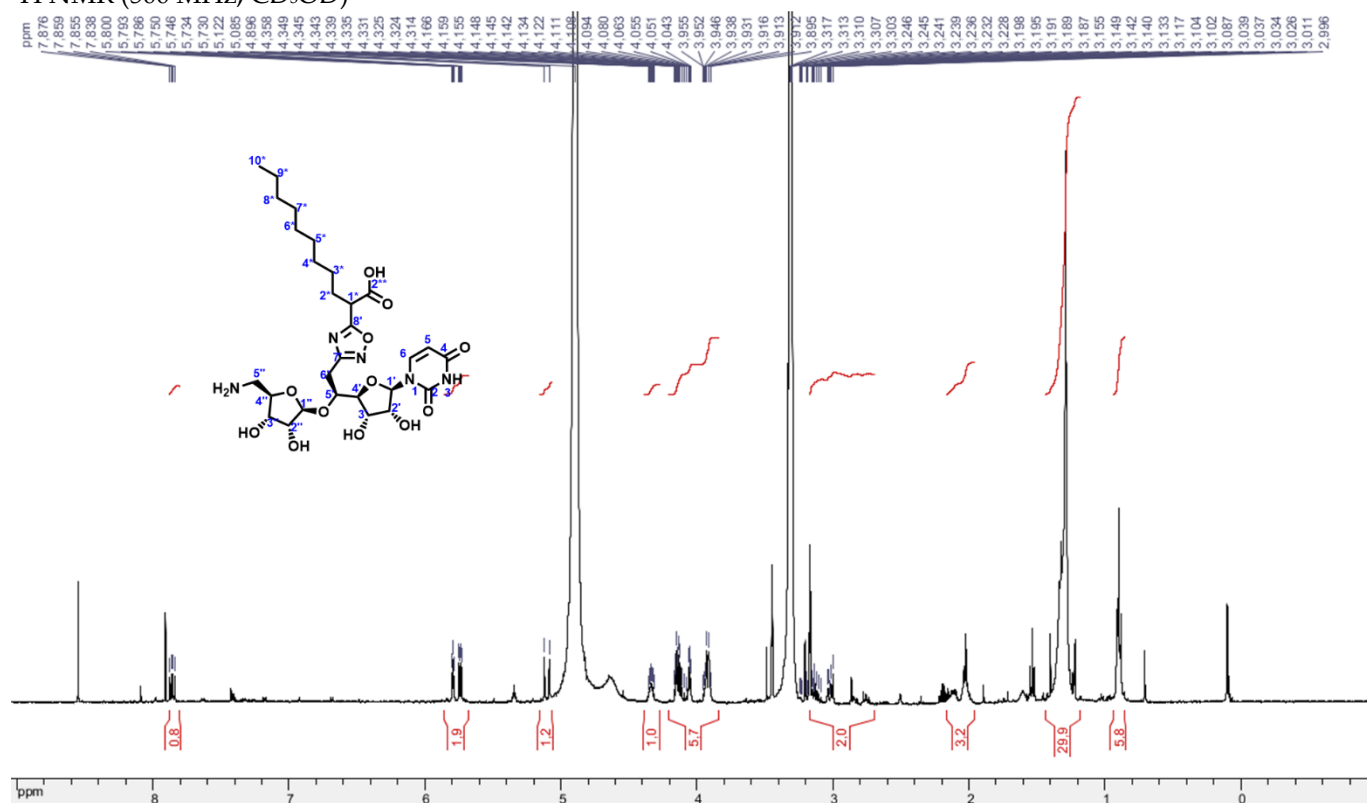


<sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)<sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)<sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)

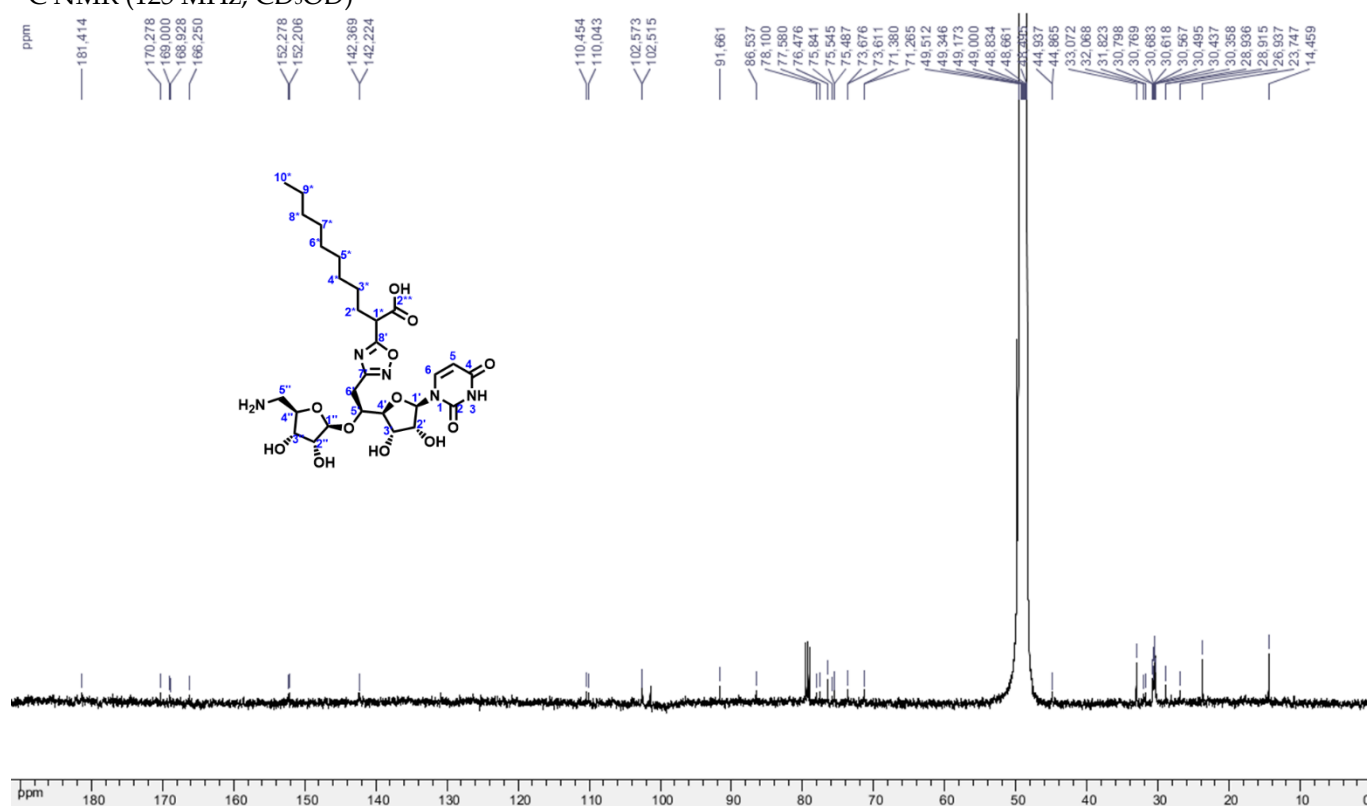


# **Oxadiazole 12j**

<sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)



<sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)



**Table S1.** Antibacterial activity of compounds **12a-12i**, and reference compounds.

Compounds	CMI ( $\mu\text{g/mL}$ )					
	Gram -			Gram +		
	<i>Escherichia coli</i> ATCC 8730	<i>Citrobacter freundii</i> ATCC 8090	<i>Pseudomonas aeruginosa</i> ATCC 27853	<i>Staphylococcus aureus</i> ATCC 25923	<i>Staphylococcus aureus</i> MRSA ATCC 43300	<i>Enterococcus faecium</i> ATCC 19434
<b>12a</b>	>50	>50	>50	>50	>50	>50
<b>12b</b>	>50	>50	>50	>50	> 50	>50
<b>12c*</b>	>50	>50	>50	50	50	50
<b>12d*</b>	>50	>50	>50	>50	>50	>50
<b>12e</b>	>50	>50	>50	>50	>50	>50
<b>12f*</b>	>50	>50	>50	50	50	50
<b>12g</b>	>50	>50	>50	>50	>50	>50
<b>12h</b>	>50	>50	>50	> 50	> 50	> 50
<b>12i*</b>	>50	>50	>50	> 50	> 50	> 50
<b>Piperacillin</b>	4	4	8	4	>128	4
<b>Vancomycin</b>	-	-	-	1	1	0.5

\* Indicates that the molecule is insoluble in 5%DMSO-water (culture media) at the highest final concentration tested