

## Supplementary Material

### Preparation of pyridine-stretched 2'-deoxyhypoxanthosine phosphoramidite

Russell Clayton,<sup>a</sup> Michael L. Davis,<sup>b</sup> Wei Li,<sup>b</sup> William Fraser,<sup>\*b</sup> and Christopher A. Ramsden<sup>\*a</sup>

<sup>a</sup>Leonard-Jones Laboratories, School of Physical and Geographical Sciences, Keele University, Keele, Staffordshire, ST5 5BG, UK

<sup>b</sup>School of Life and Health Sciences, Aston University, Aston Triangle, Birmingham, B4 7ET, UK

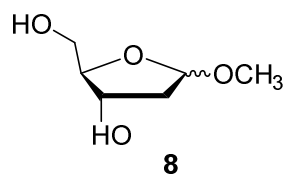
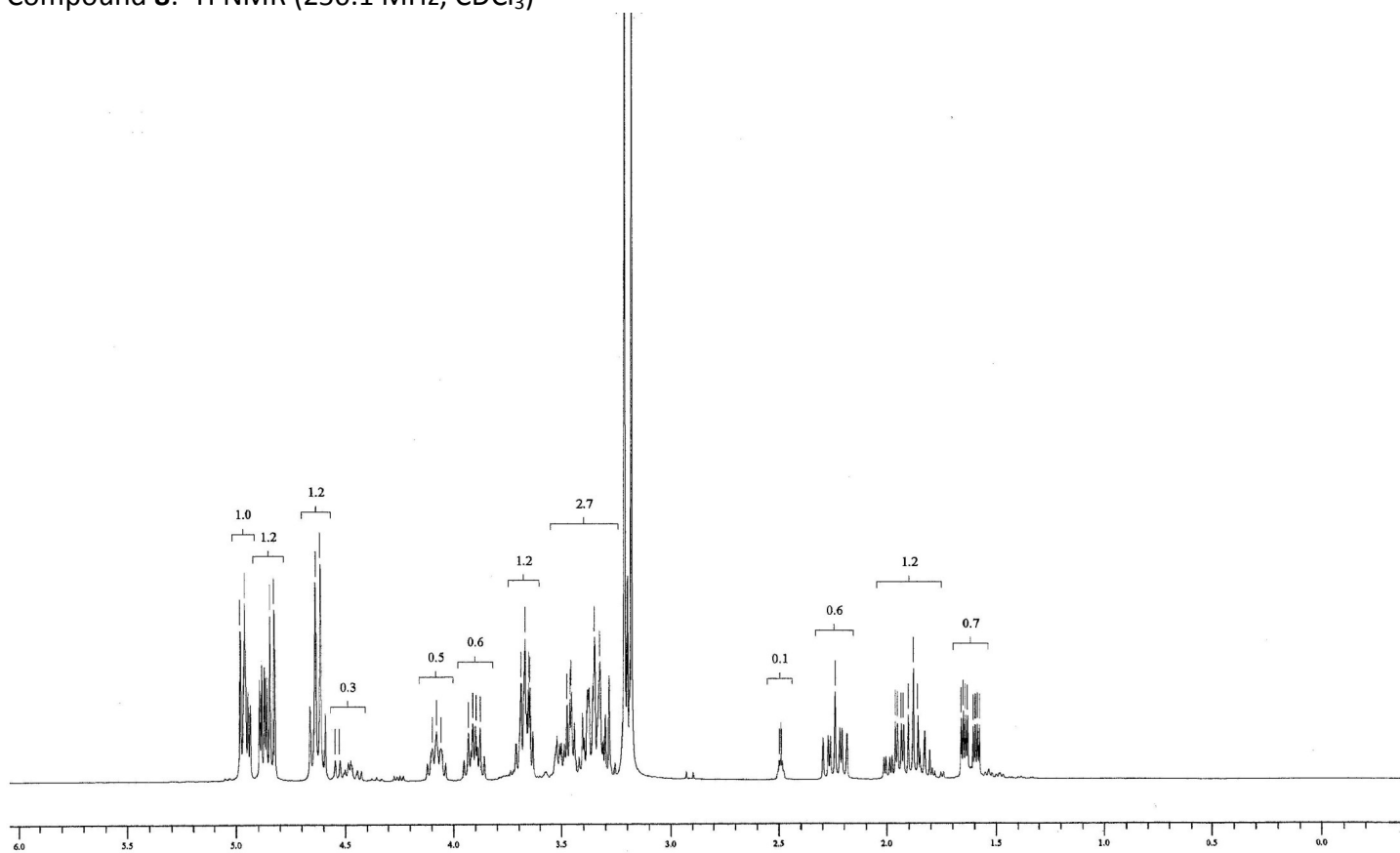
Email: [w.fraser@aston.ac.uk](mailto:w.fraser@aston.ac.uk), [c.a.ramsden@keele.ac.uk](mailto:c.a.ramsden@keele.ac.uk)

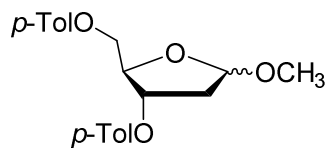
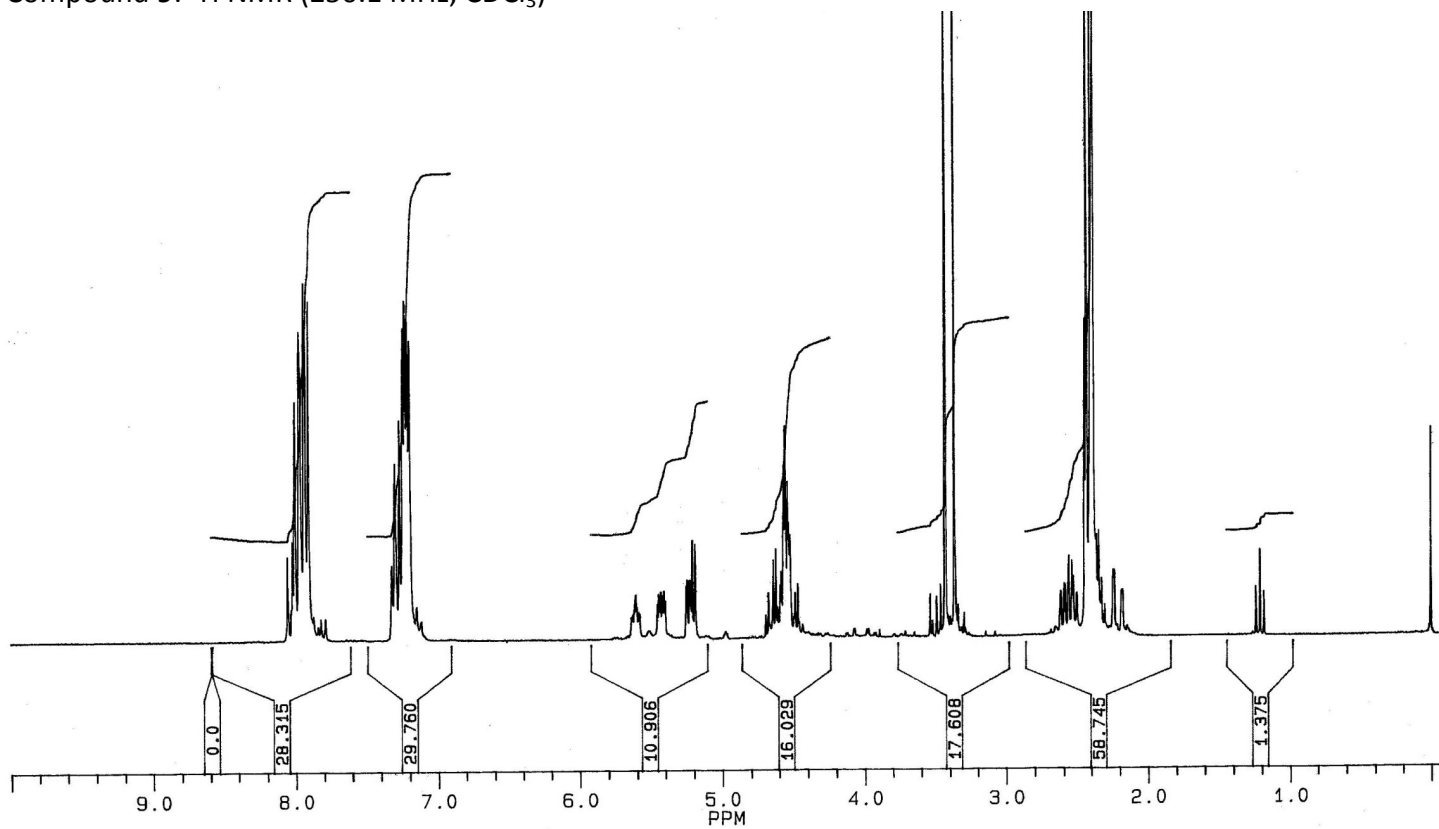
#### Table of Contents

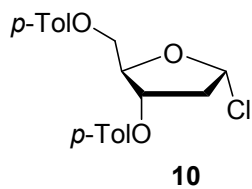
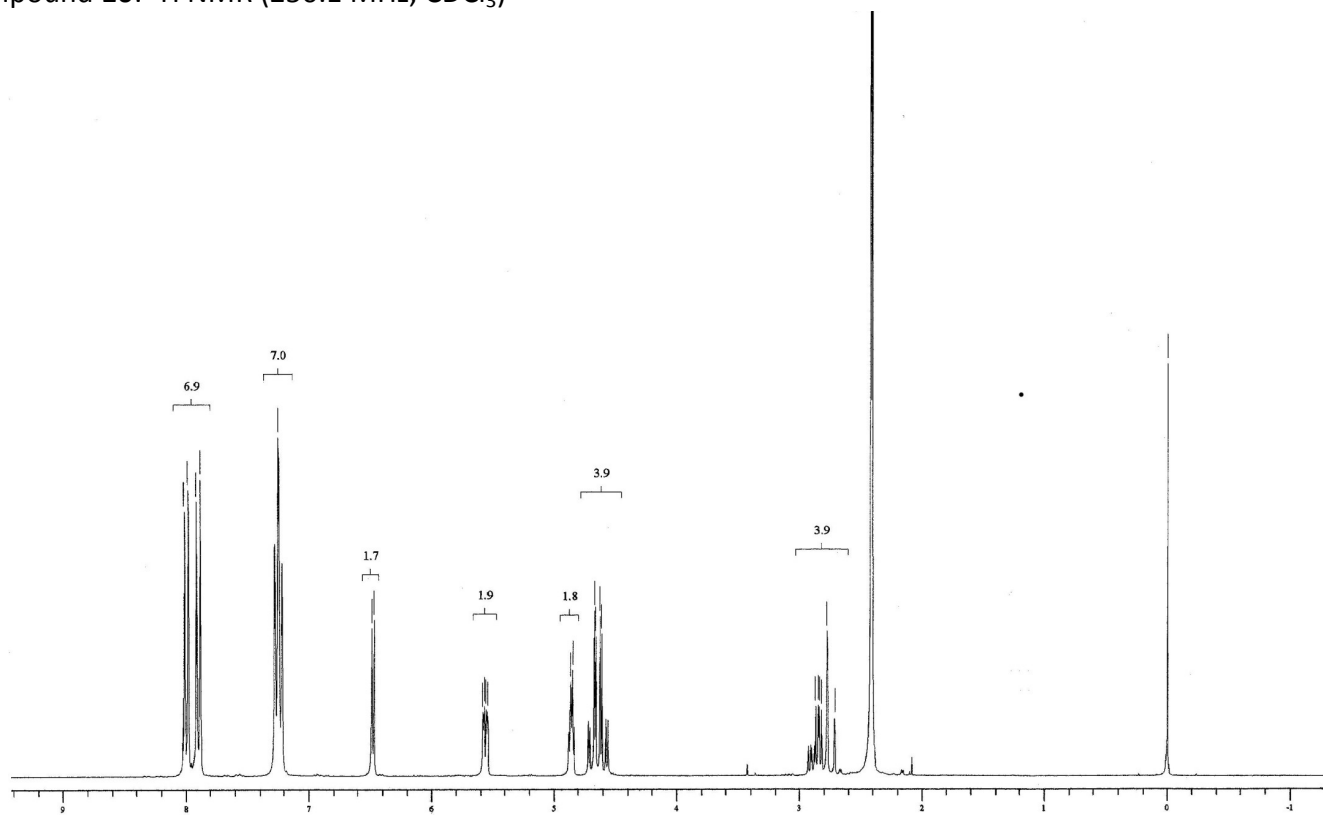
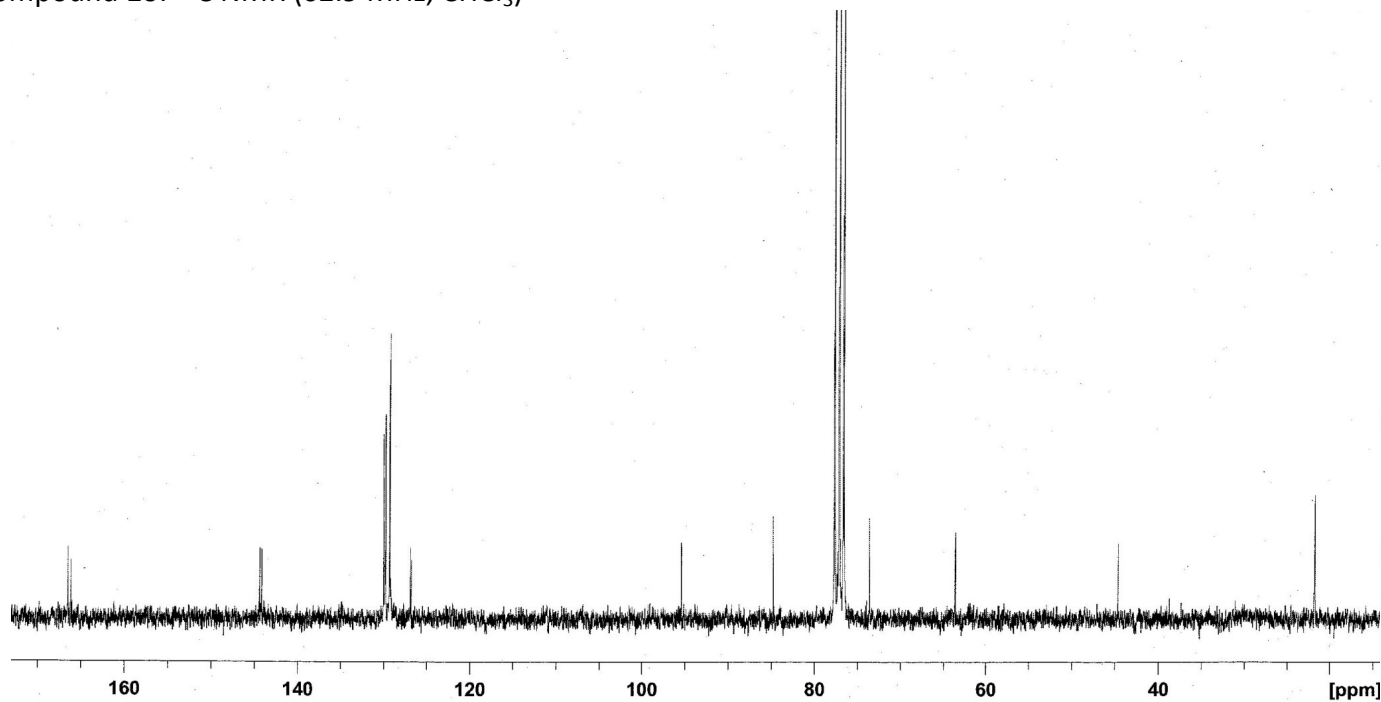
Compound <b>8</b> : <sup>1</sup> H NMR (250.1 MHz, CDCl <sub>3</sub> )	S3
Compound <b>9</b> : <sup>1</sup> H NMR (250.1 MHz, CDCl <sub>3</sub> )	S4
Compound <b>10</b> : <sup>1</sup> H NMR (250.1 MHz, CDCl <sub>3</sub> )	S5
Compound <b>10</b> : <sup>13</sup> C NMR (62.9 MHz, CDCl <sub>3</sub> )	S5
Compound <b>12</b> : <sup>1</sup> H NMR (250.1 MHz, DMSO- <i>d</i> <sub>6</sub> )	S6
Compound <b>12</b> : <sup>13</sup> C NMR (62.9 MHz, DMSO- <i>d</i> <sub>6</sub> )	S6
Compound <b>13</b> : <sup>1</sup> H NMR (250.1 MHz, DMSO- <i>d</i> <sub>6</sub> )	S7
Compound <b>13</b> : <sup>13</sup> C NMR (62.9 MHz, DMSO- <i>d</i> <sub>6</sub> )	S7
Compound <b>14</b> : <sup>1</sup> H NMR (250.1 MHz, DMSO- <i>d</i> <sub>6</sub> )	S8
Compound <b>14</b> : <sup>13</sup> C NMR (62.9 MHz, DMSO- <i>d</i> <sub>6</sub> )	S8
Compound <b>15</b> : <sup>1</sup> H NMR (250.1 MHz, CDCl <sub>3</sub> )	S9
Compound <b>15</b> : <sup>13</sup> C NMR (62.9 MHz, CDCl <sub>3</sub> )	S9
Compound <b>15</b> : NOESY (400.1 MHz, CDCl <sub>3</sub> )	S10
Compound <b>16</b> : <sup>1</sup> H NMR (250.1 MHz, CDCl <sub>3</sub> )	S11
Compound <b>16</b> : <sup>13</sup> C NMR (62.9 MHz, CDCl <sub>3</sub> )	S11
Compound <b>18</b> : <sup>1</sup> H NMR (250.1 MHz, CDCl <sub>3</sub> )	S12
Compound <b>18</b> : <sup>13</sup> C NMR (62.9 MHz, CDCl <sub>3</sub> )	S12
Compound <b>19</b> : <sup>1</sup> H NMR (400.1 MHz, DMSO- <i>d</i> <sub>6</sub> )	S13
Compound <b>19</b> : <sup>13</sup> C NMR (62.9 MHz, DMSO- <i>d</i> <sub>6</sub> )	S13
Compound <b>19</b> : NOESY (400.1 MHz, DMSO- <i>d</i> <sub>6</sub> )	S14
Compound <b>20</b> : <sup>1</sup> H NMR (250.1 MHz, DMSO- <i>d</i> <sub>6</sub> )	S15
Compound <b>20</b> : <sup>13</sup> C NMR (62.9 MHz, DMSO- <i>d</i> <sub>6</sub> )	S15
Compound <b>20</b> : NOESY (400.1 MHz, DMSO- <i>d</i> <sub>6</sub> )	S16
Compound <b>21</b> : <sup>1</sup> H NMR (250.1 MHz, THF- <i>d</i> <sub>8</sub> )	S17
Compound <b>22</b> : <sup>1</sup> H NMR (250.1 MHz, DMSO- <i>d</i> <sub>6</sub> )	S18
Compound <b>22</b> : <sup>13</sup> C NMR (62.9 MHz, DMSO- <i>d</i> <sub>6</sub> )	S18
Compound <b>23</b> : <sup>1</sup> H NMR (400.1 MHz, CDCl <sub>3</sub> )	S19
Compound <b>23</b> : <sup>13</sup> C NMR (101.6 MHz, CDCl <sub>3</sub> )	S19
Compound <b>26</b> : <sup>1</sup> H NMR (400.1 MHz, CDCl <sub>3</sub> )	S20

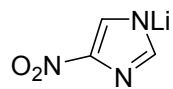
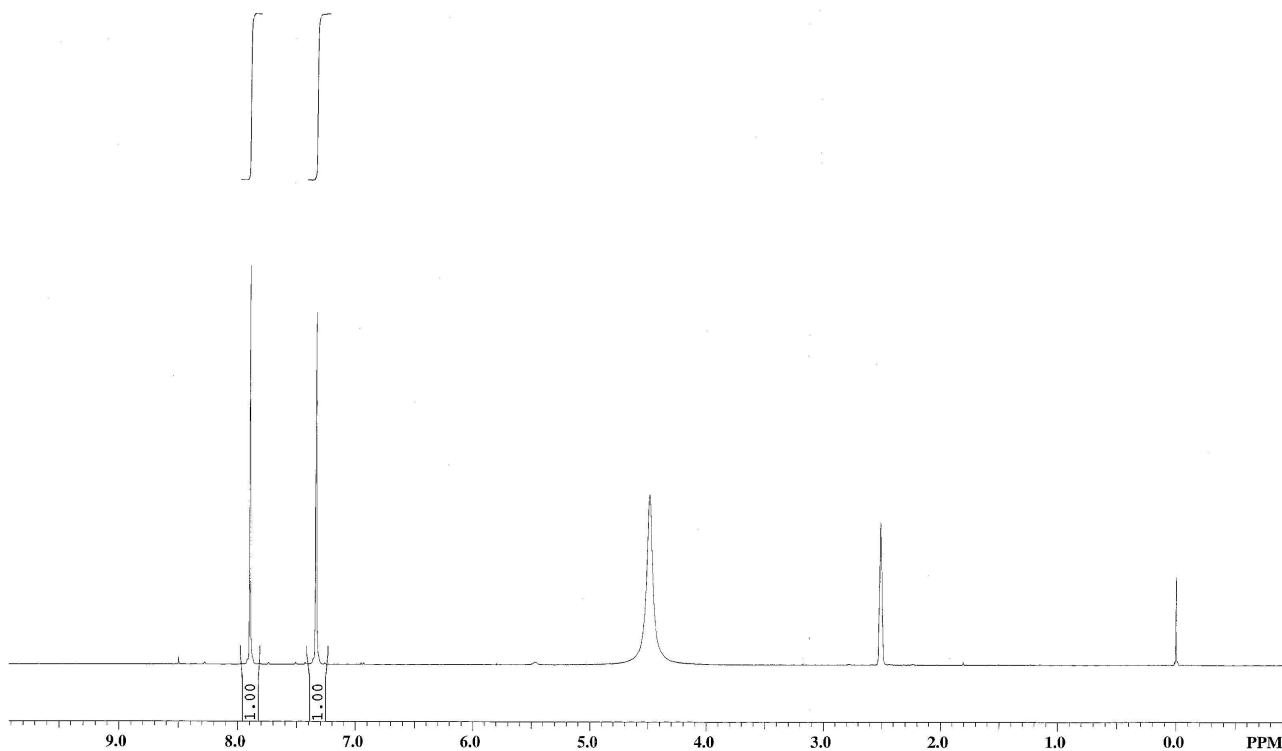
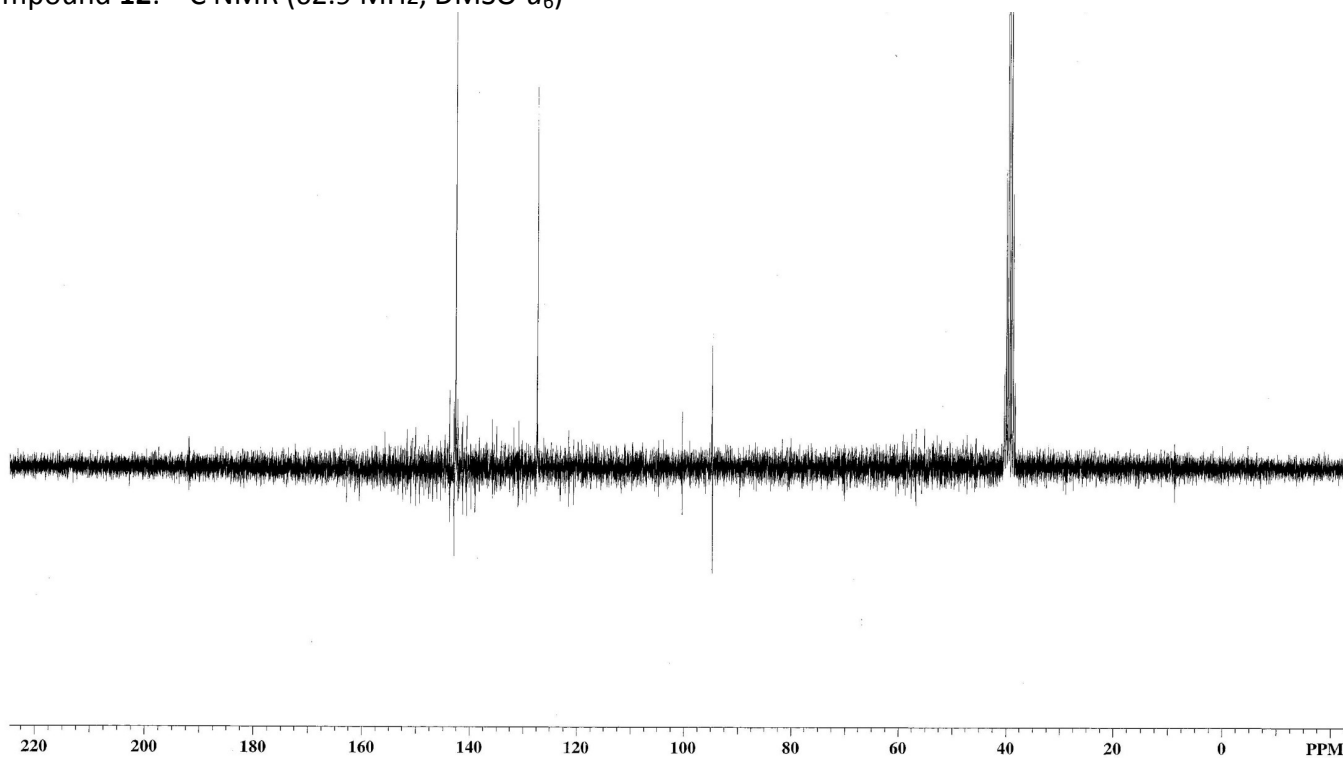
## Table of Contents Continued

Compound <b>26</b> : $^{13}\text{C}$ NMR (101.6 MHz, $\text{CDCl}_3$ )	S20
Compound <b>24</b> : $^1\text{H}$ NMR (250.1 MHz, $\text{DMSO-}d_6$ )	S21
Compound <b>24</b> : $^{13}\text{C}$ NMR (62.9 MHz, $\text{DMSO-}d_6$ )	S21
Compound <b>27</b> : $^1\text{H}$ NMR (250.1 MHz, $\text{DMSO-}d_6$ )	S22
Compound <b>27</b> : $^{13}\text{C}$ NMR (62.9 MHz, $\text{DMSO-}d_6$ )	S22
Compound <b>5</b> : $^1\text{H}$ NMR (250.1 MHz, $\text{DMSO-}d_6$ )	S23
Compound <b>5</b> : $^{13}\text{C}$ NMR (62.9 MHz, $\text{DMSO-}d_6$ )	S23
Compound <b>28</b> : $^1\text{H}$ NMR (250.1 MHz, $\text{DMSO-}d_6$ )	S24
Compound <b>28</b> : $^{13}\text{C}$ NMR (62.9 MHz, $\text{DMSO-}d_6$ )	S24
Compound <b>30</b> : $^1\text{H}$ NMR (250.1 MHz, $\text{DMSO-}d_6$ )	S25
Compound <b>4</b> : $^1\text{H}$ NMR (250.1 MHz, $\text{DMSO-}d_6$ )	S26
Compound <b>4</b> : $^{13}\text{C}$ NMR (62.9 MHz, $\text{DMSO-}d_6$ )	S26
Compound <b>31</b> : $^1\text{H}$ NMR (250.1 MHz, $\text{DMSO-}d_6$ )	S27
Compound <b>31</b> : $^{13}\text{C}$ NMR (62.9 MHz, $\text{DMSO-}d_6$ )	S27

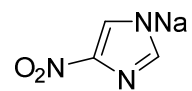
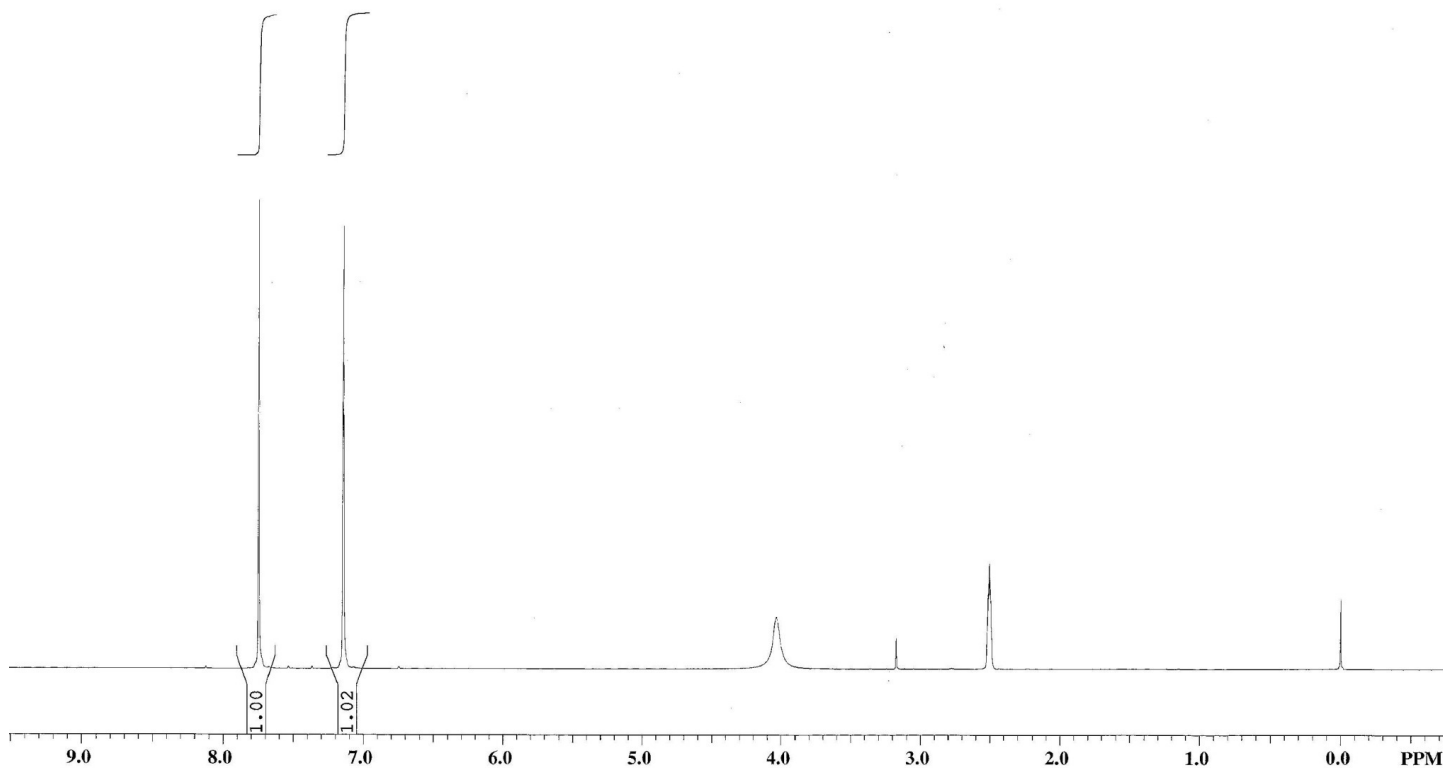
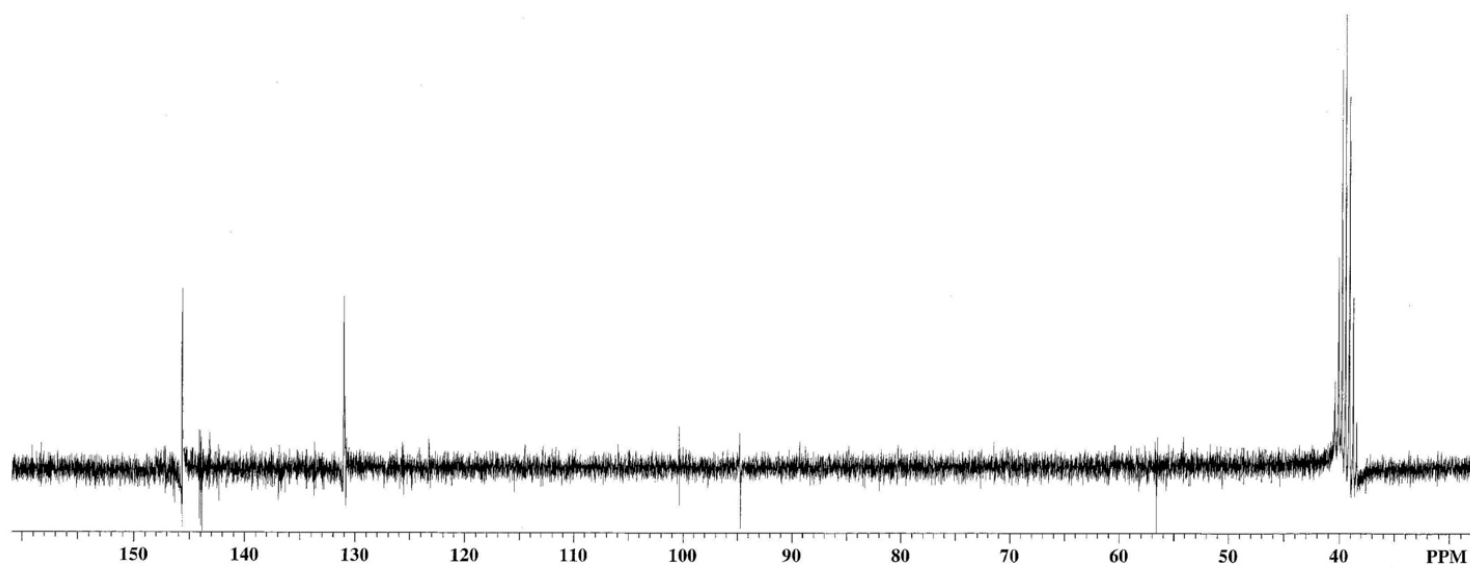
Compound **8**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{CDCl}_3$ )

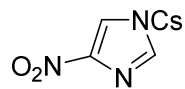
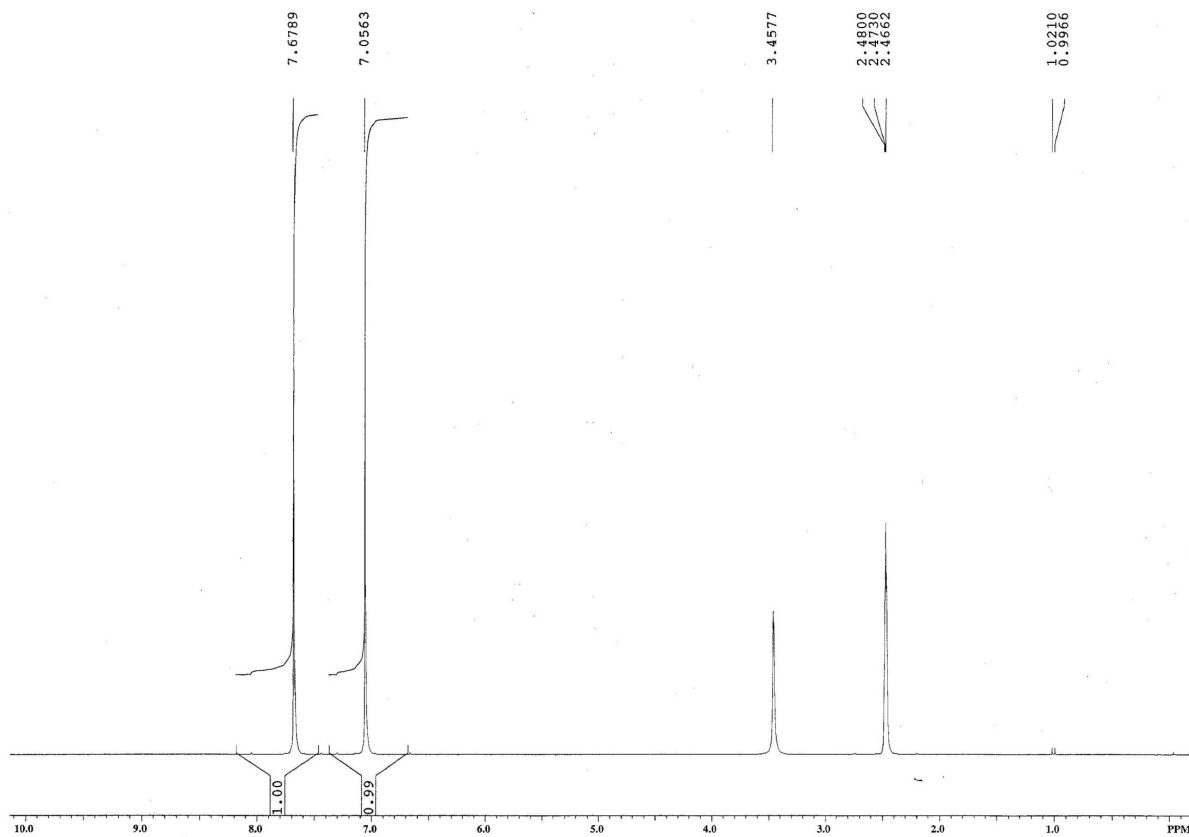
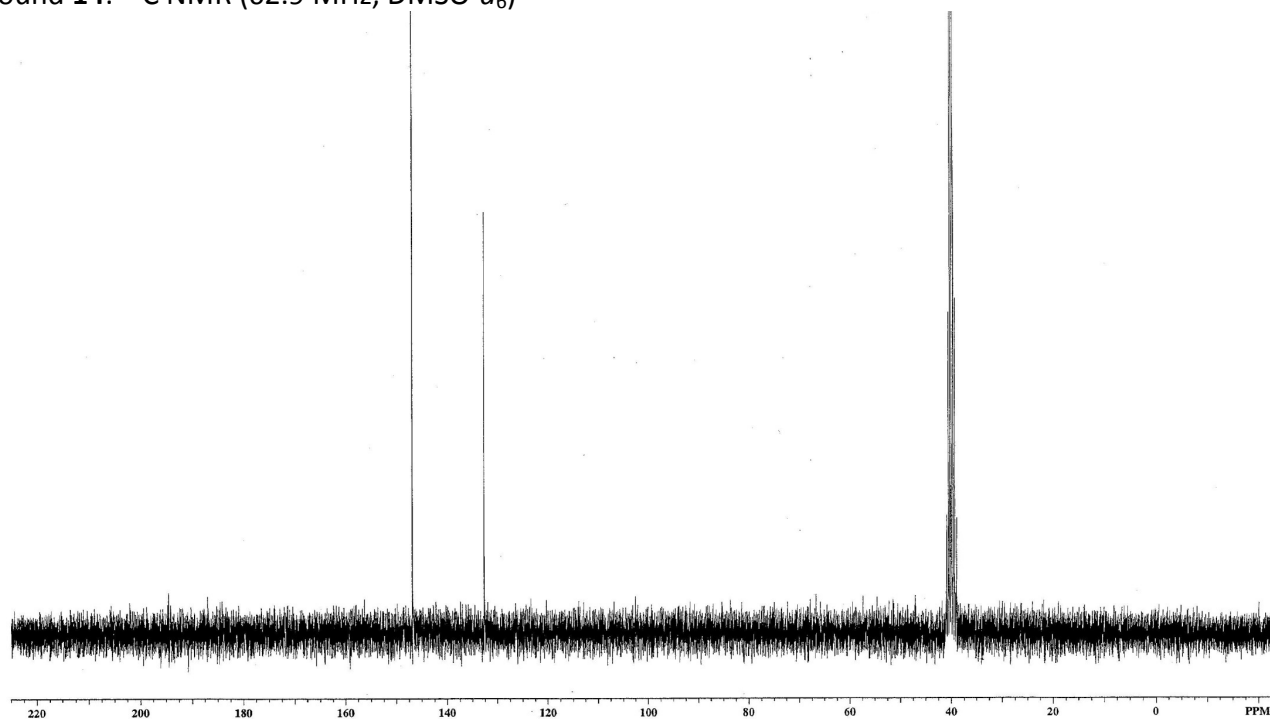
**9**Compound **9**: <sup>1</sup>H NMR (250.1 MHz, CDCl<sub>3</sub>)

Compound **10**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{CDCl}_3$ )Compound **10**:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{CHCl}_3$ )

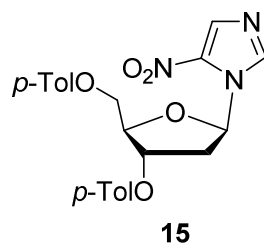
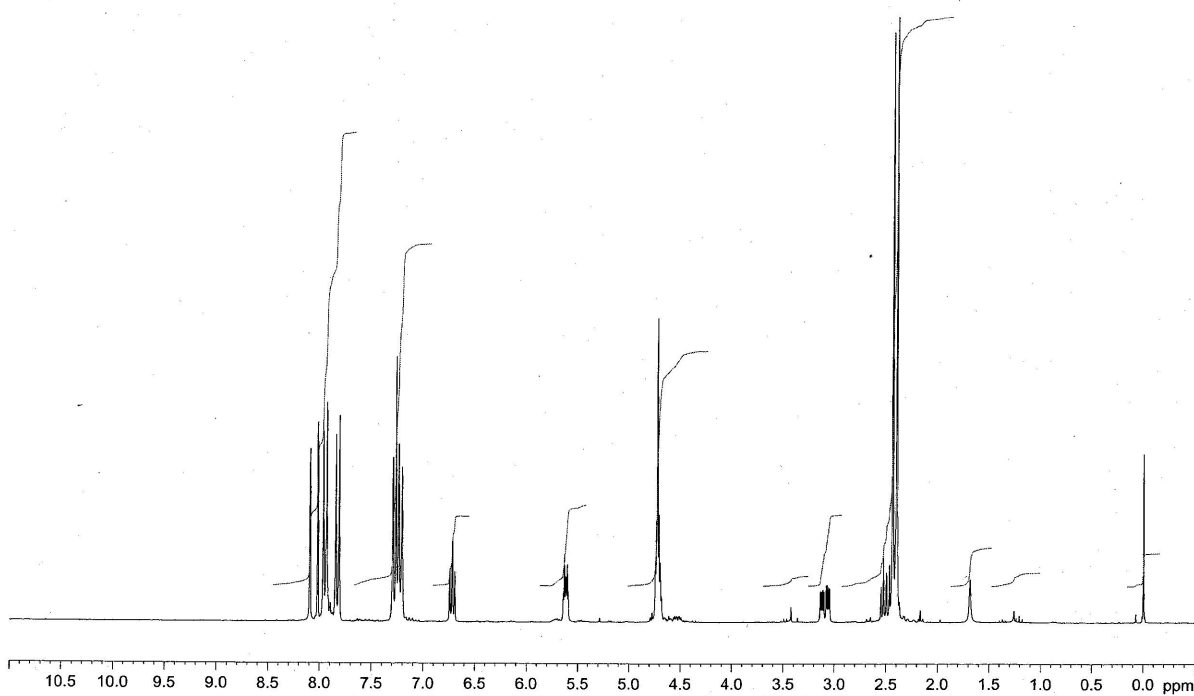
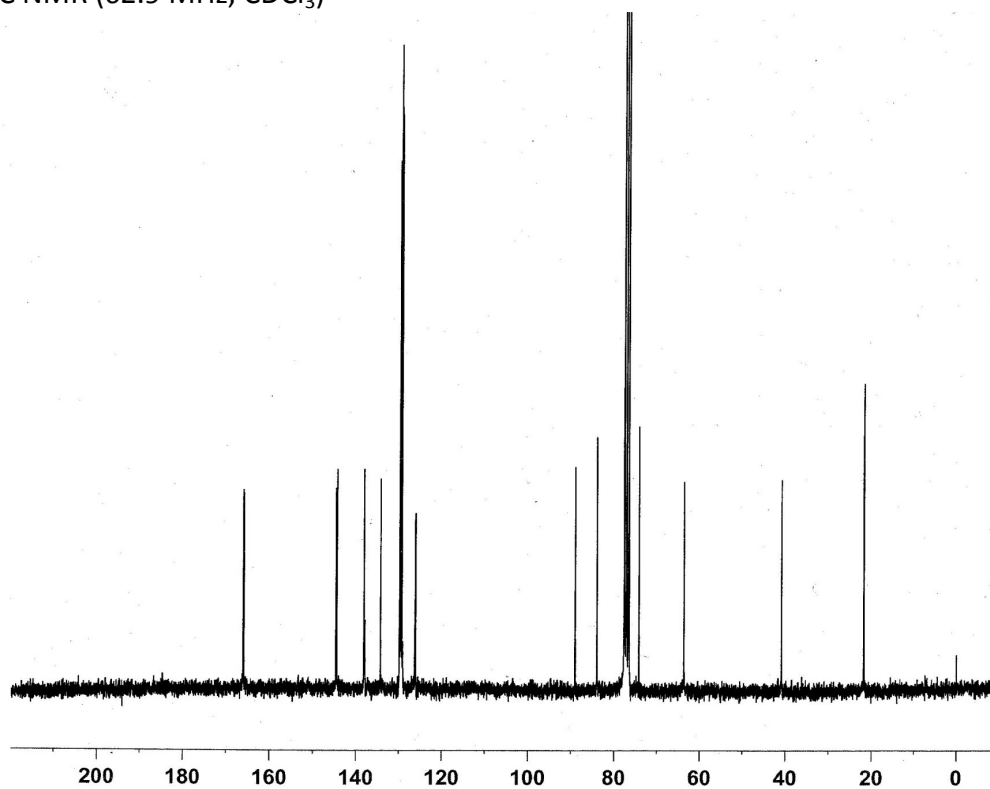
**12**Compound **12**:  $^1\text{H}$  NMR (250.1 MHz, DMSO- $d_6$ )Compound **12**:  $^{13}\text{C}$  NMR (62.9 MHz, DMSO- $d_6$ )

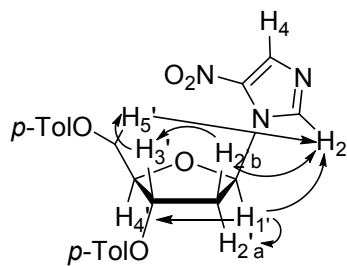
§

**13**Compound **13**:  $^1\text{H}$  NMR (250.1 MHz, DMSO- $d_6$ )Compound **13**:  $^{13}\text{C}$  NMR (62.9 MHz, DMSO- $d_6$ )

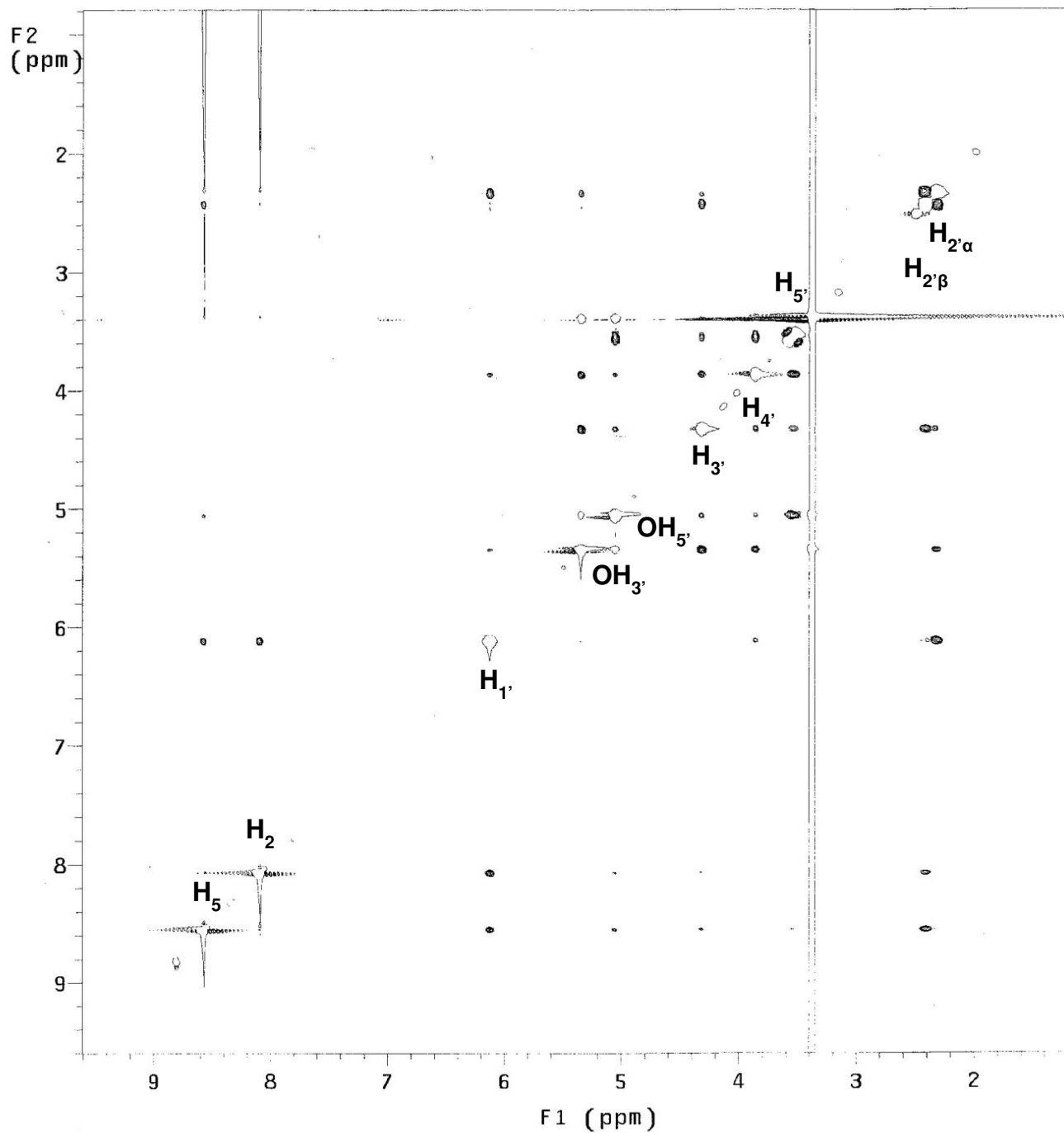
**14**Compound **14**:  $^1\text{H}$  NMR (250.1 MHz, DMSO- $d_6$ )Compound **14**:  $^{13}\text{C}$  NMR (62.9 MHz, DMSO- $d_6$ )

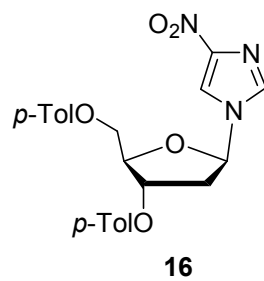
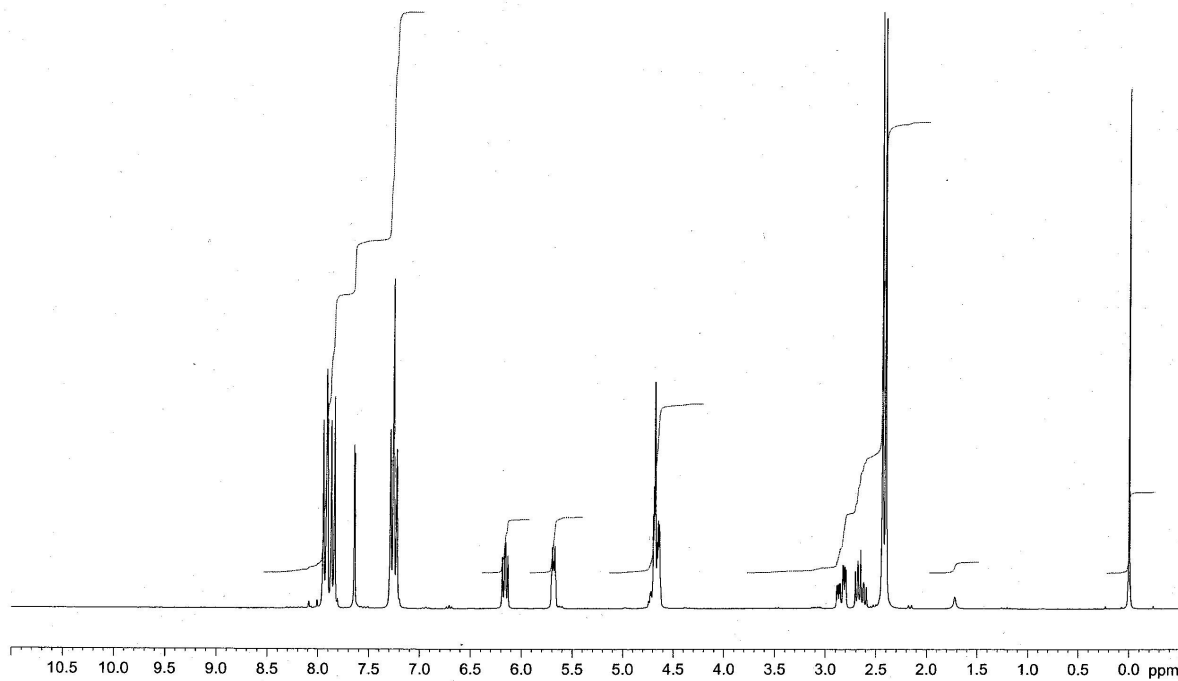
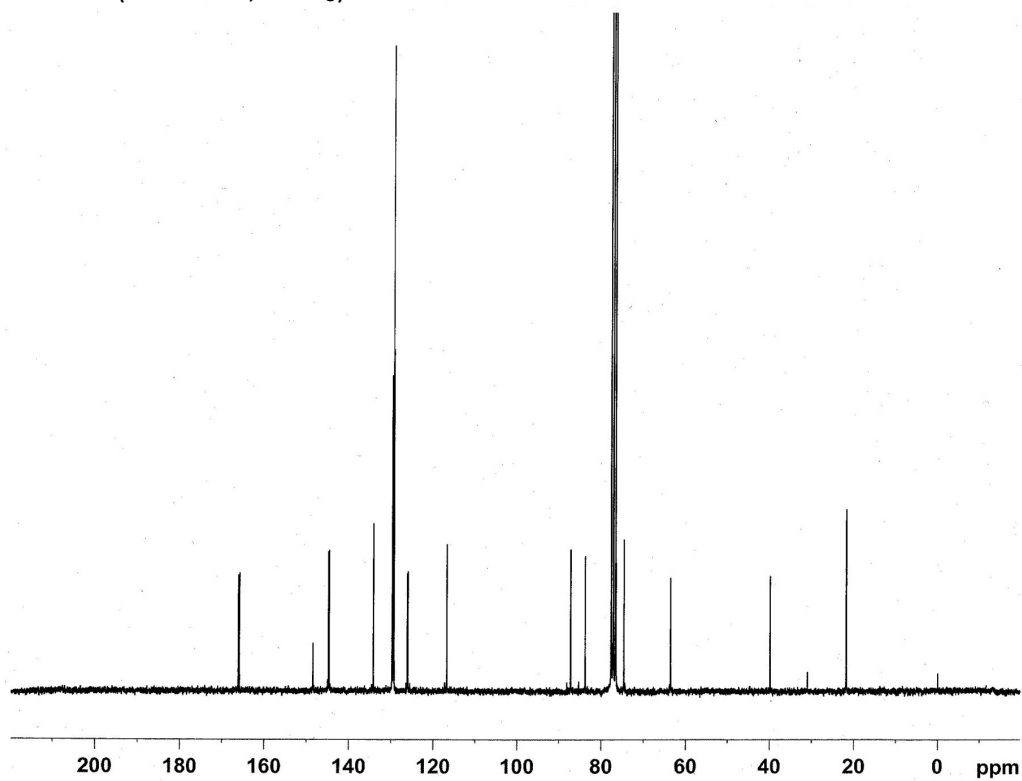


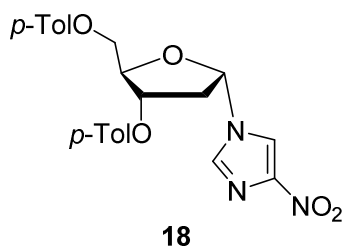
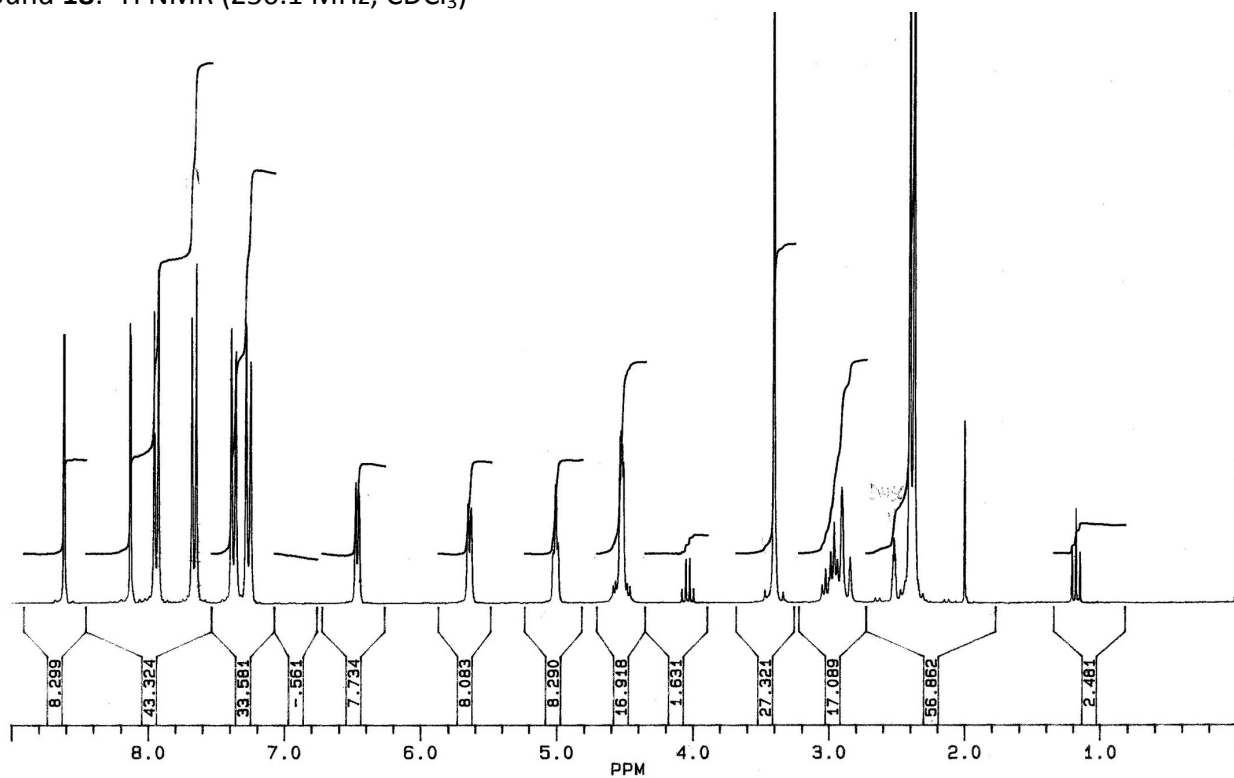
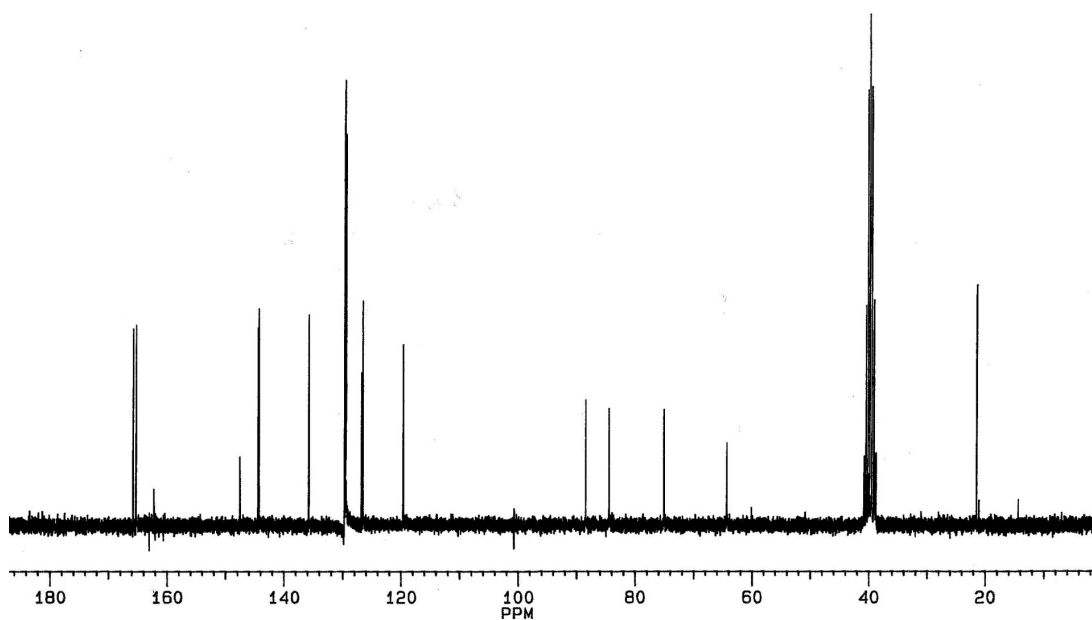
**15**Compound **15**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{CDCl}_3$ )Compound **15**:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{CDCl}_3$ )

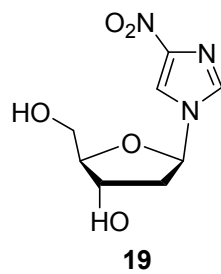
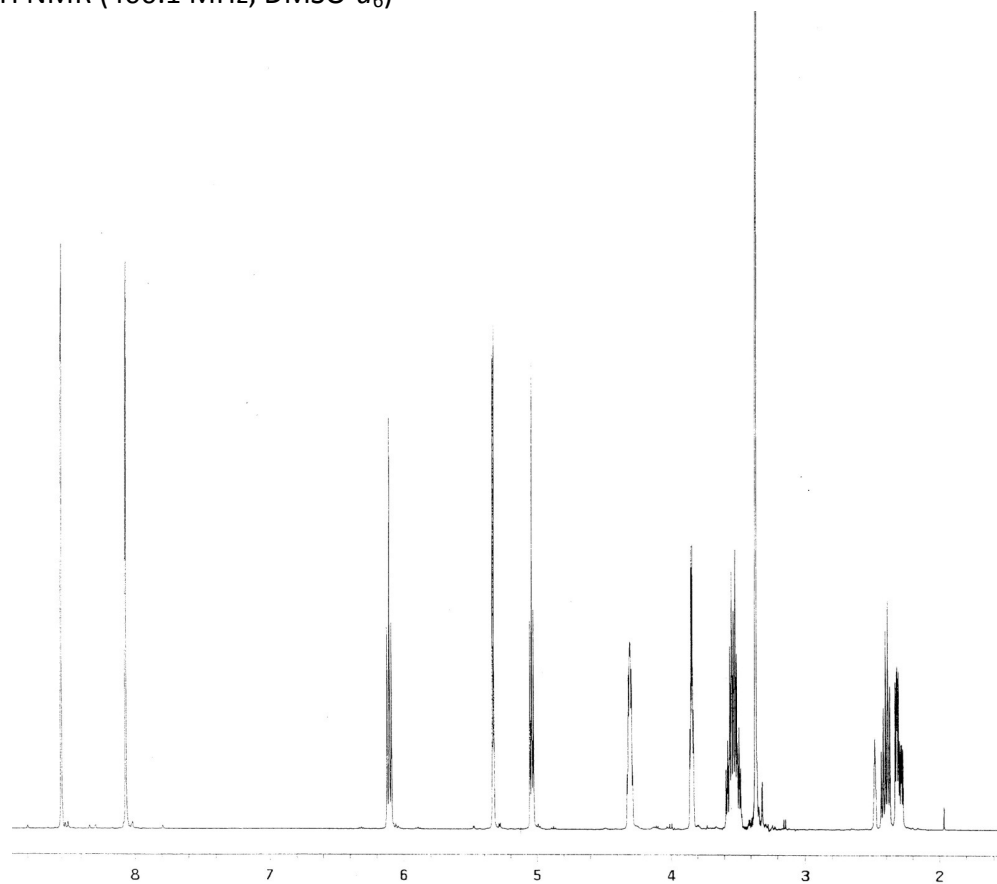
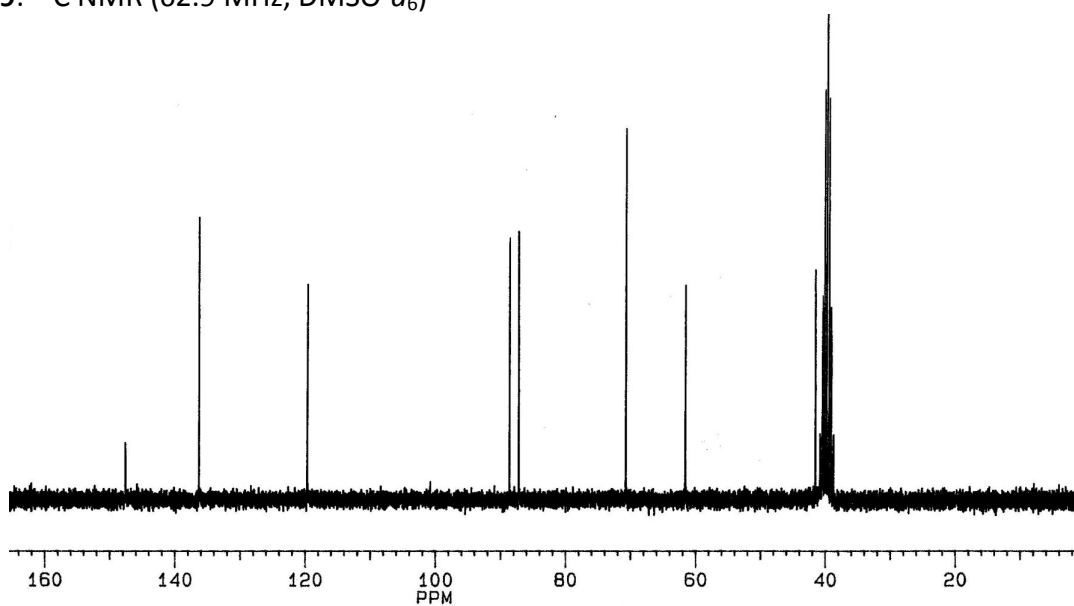


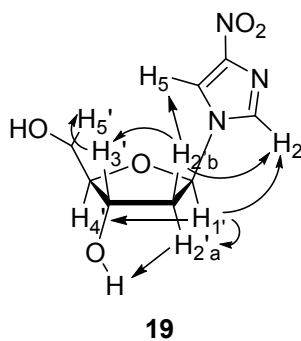
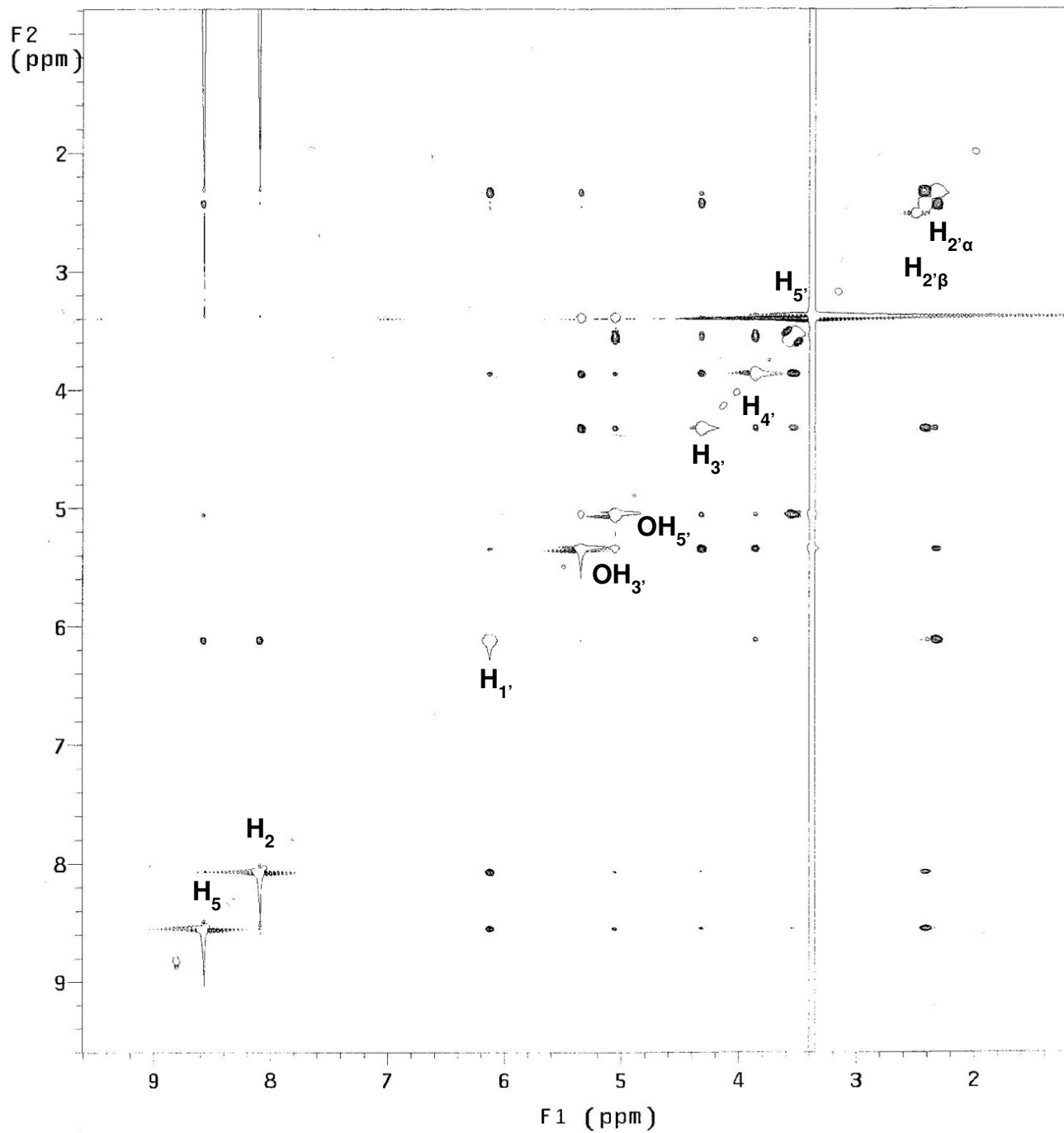
15

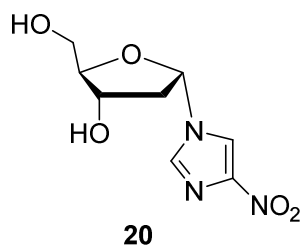
Compound 15: NOESY (400.1 MHz, CDCl<sub>3</sub>)

Compound **16**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{CDCl}_3$ )Compound **16**:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{CDCl}_3$ )

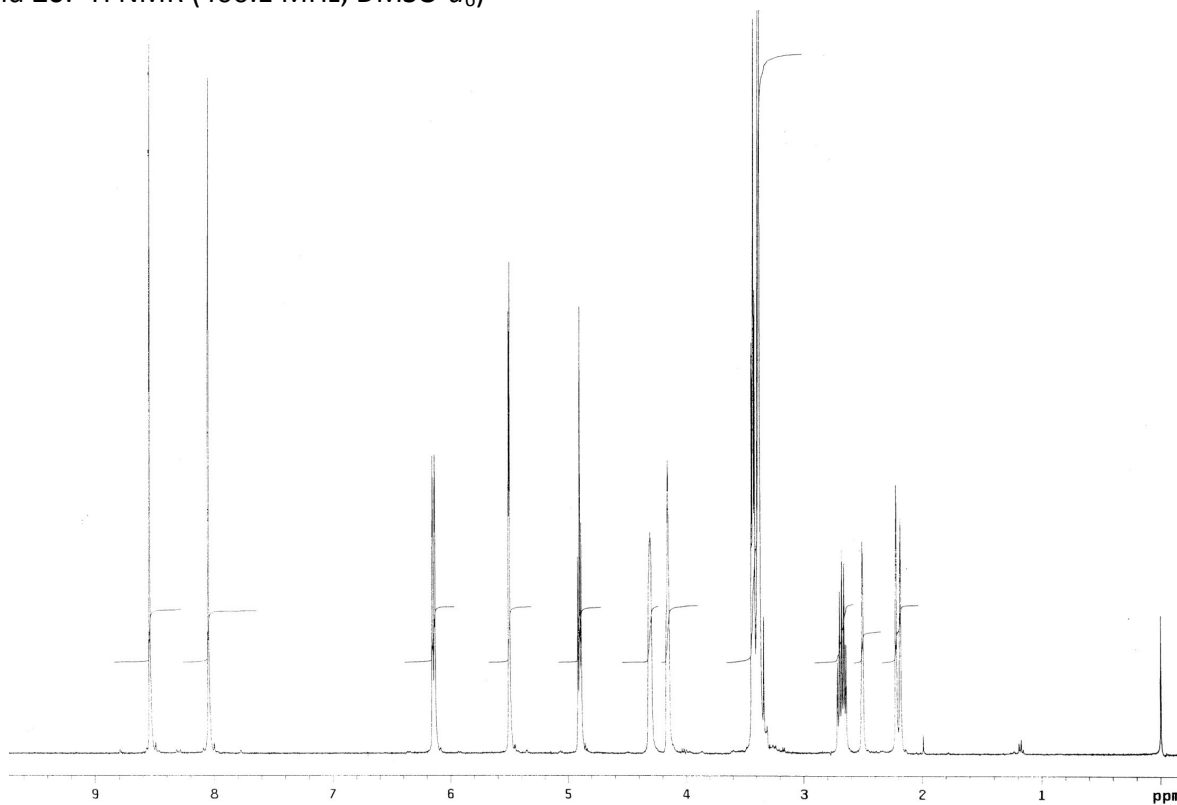
Compound **18**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{CDCl}_3$ )Compound **18**:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{CDCl}_3$ )

Compound 19:  $^1\text{H}$  NMR (400.1 MHz,  $\text{DMSO-}d_6$ )Compound 19:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{DMSO-}d_6$ )

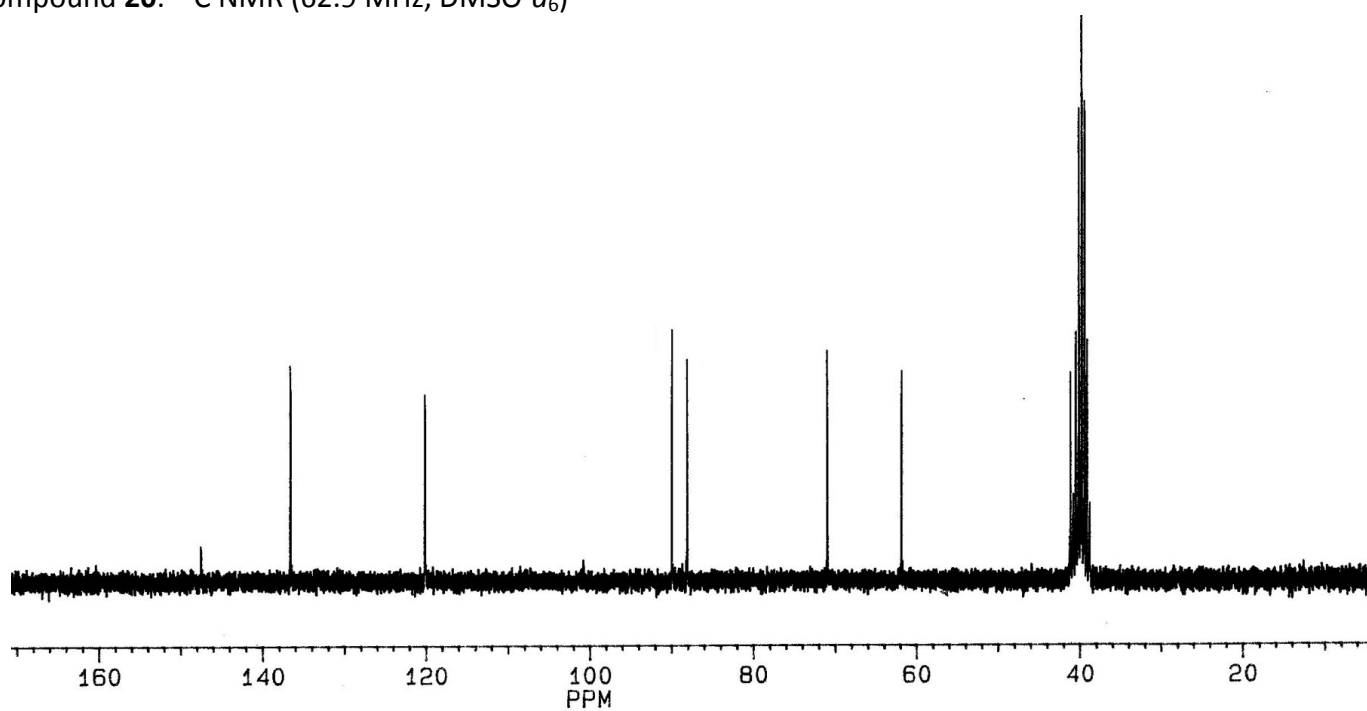
Compound **19**: NOESY (400.1 MHz, DMSO-*d*<sub>6</sub>)

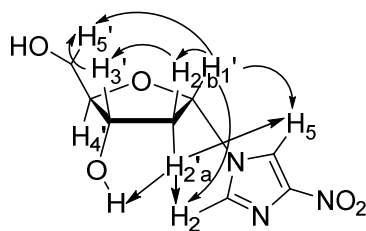


Compound **20**:  $^1\text{H}$  NMR (400.1 MHz,  $\text{DMSO-}d_6$ )

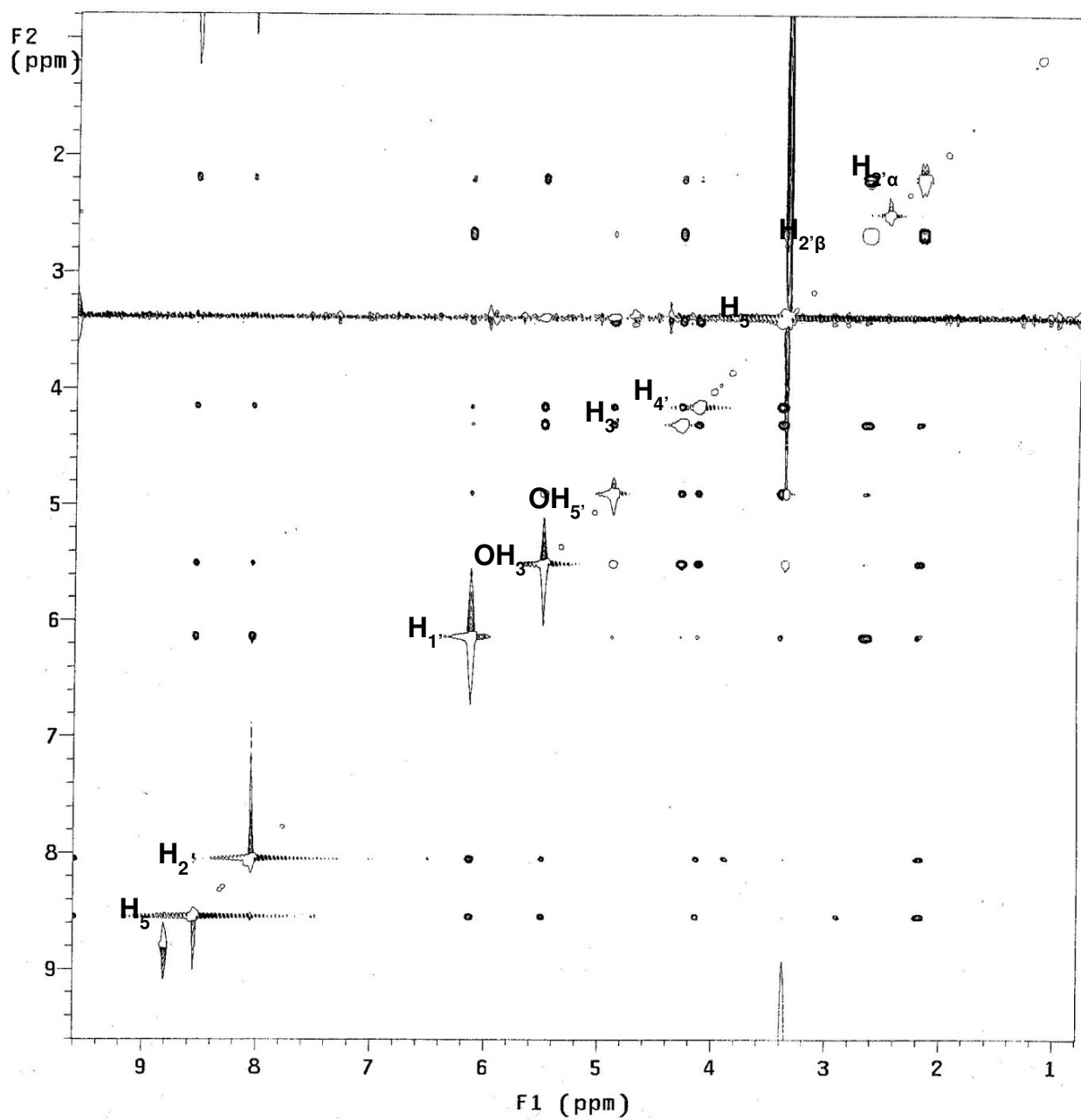


Compound **20**:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{DMSO-}d_6$ )

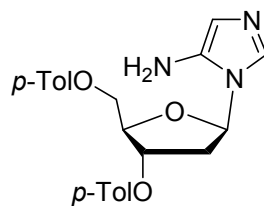




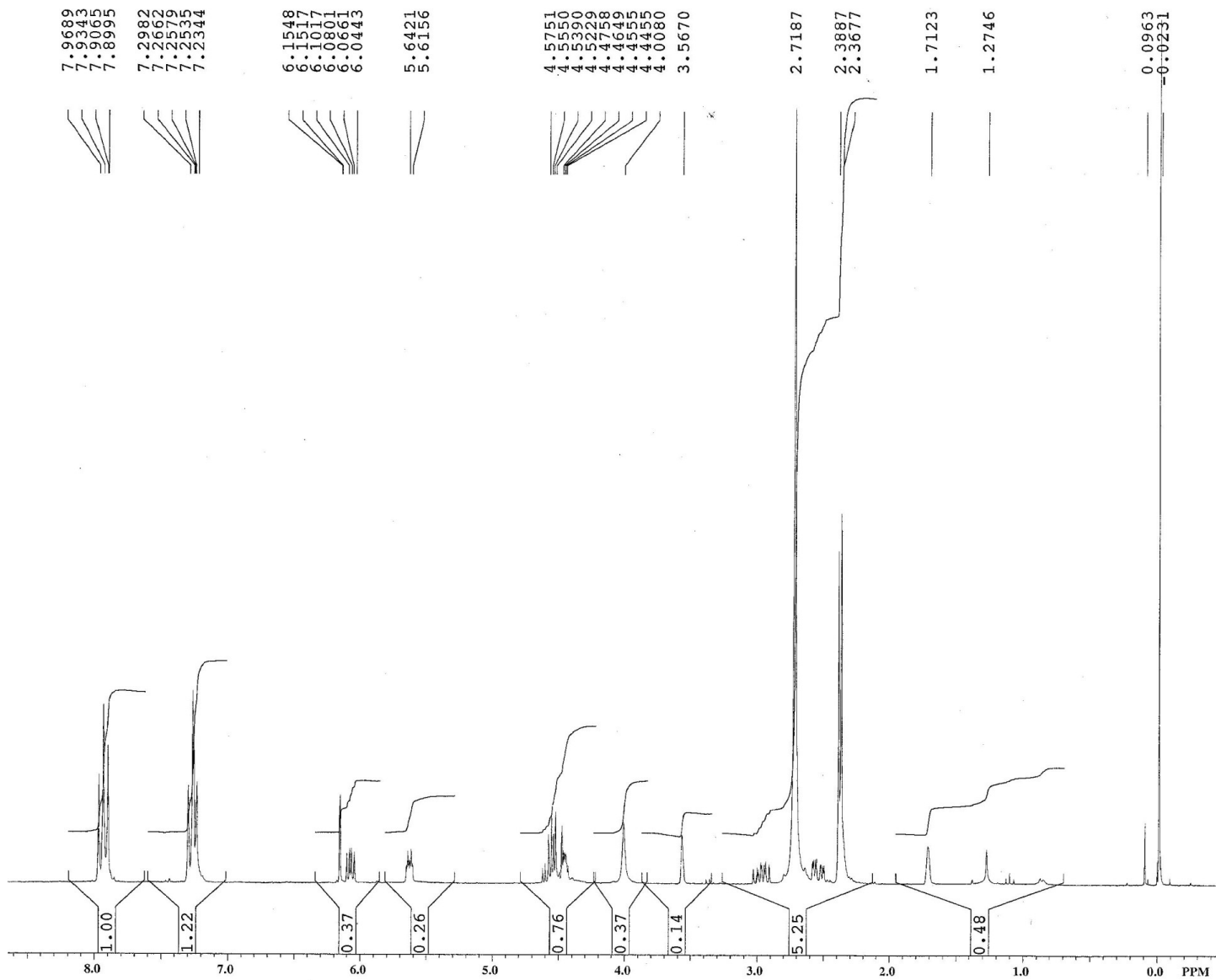
20

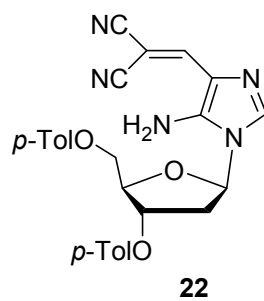
Compound 20: NOESY (400.1 MHz, DMSO- $d_6$ )



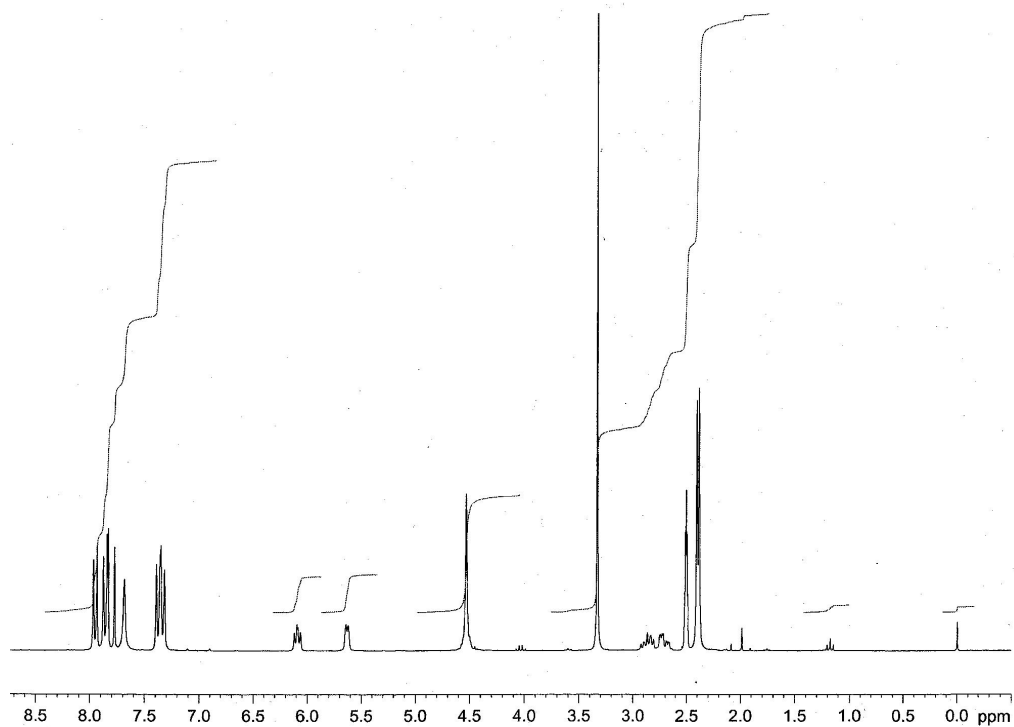


Compound **21**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{THF-}d_8$ )

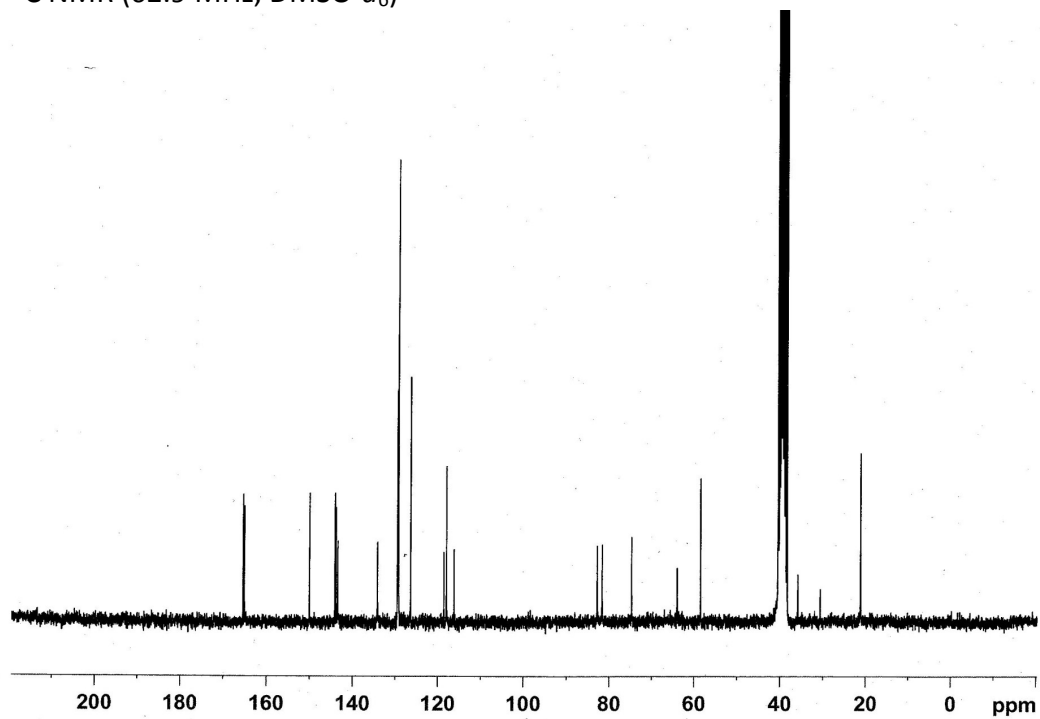


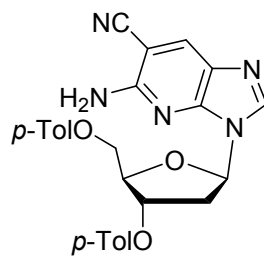
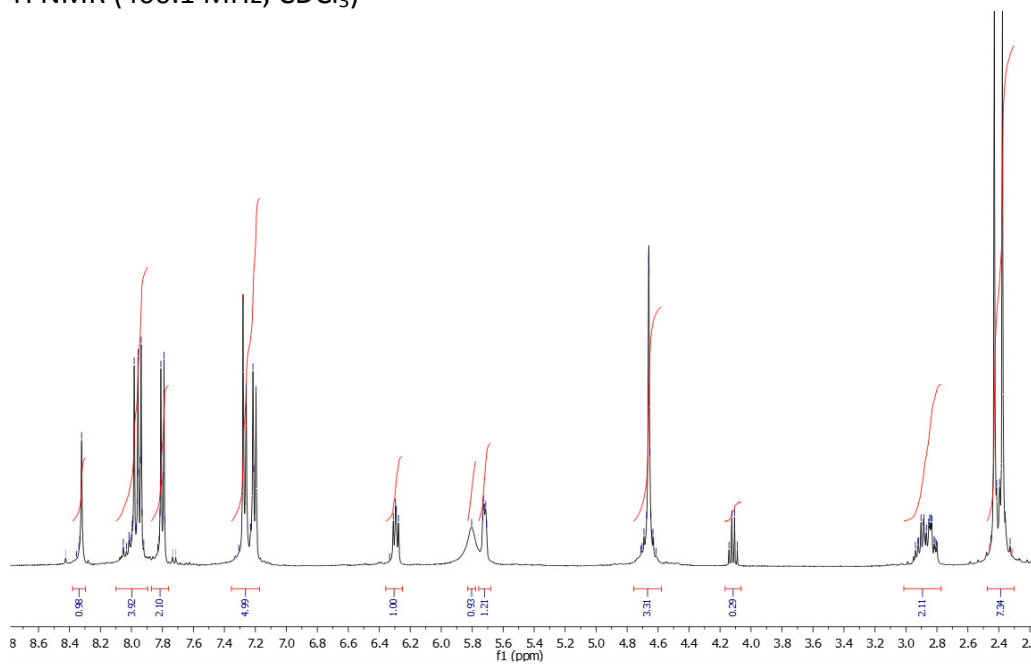
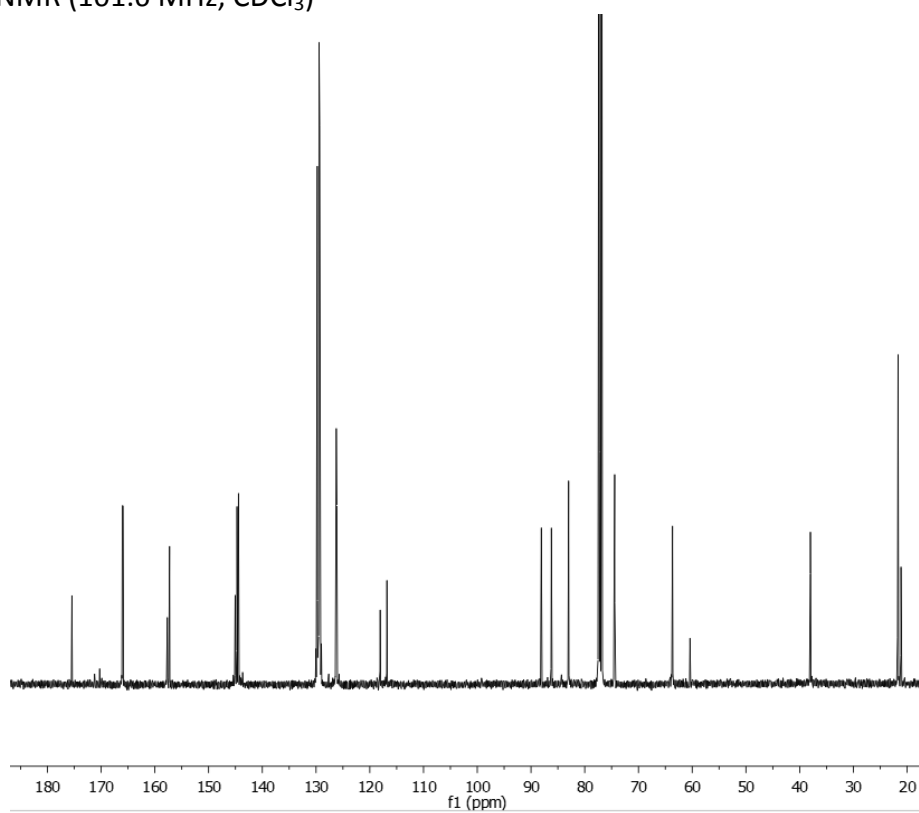
**22**

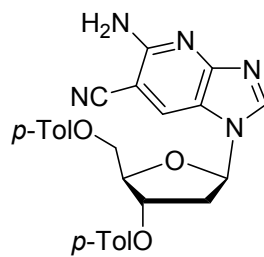
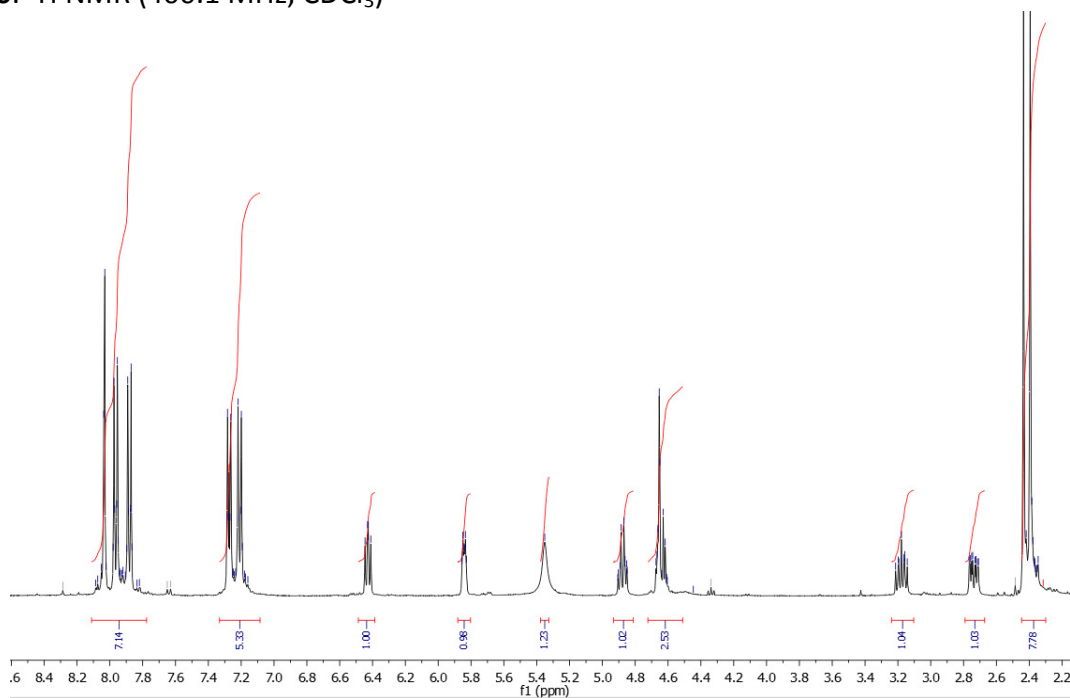
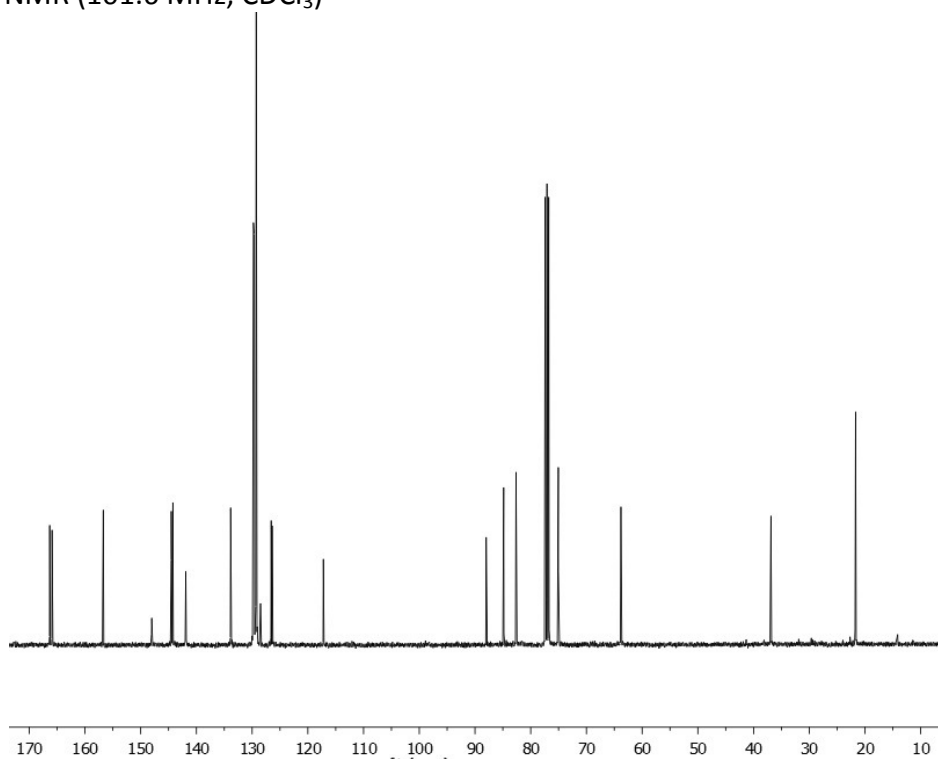
Compound **22**: <sup>1</sup>H NMR (250.1 MHz, DMSO-*d*<sub>6</sub>)

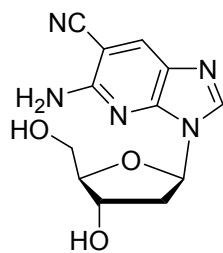
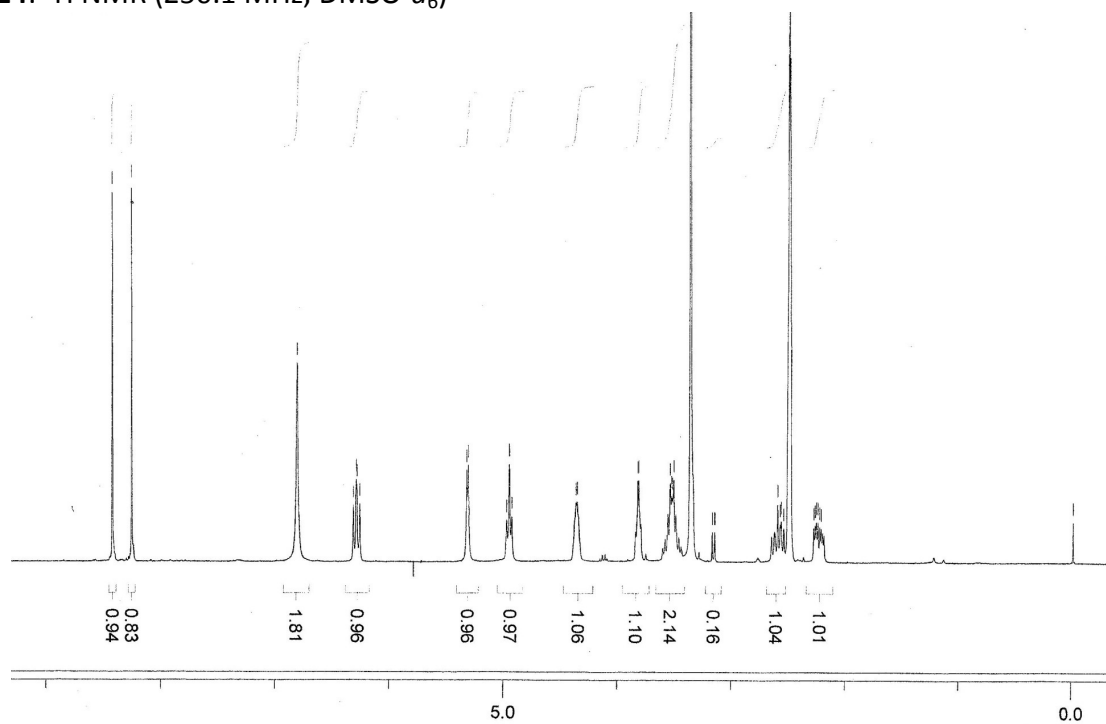
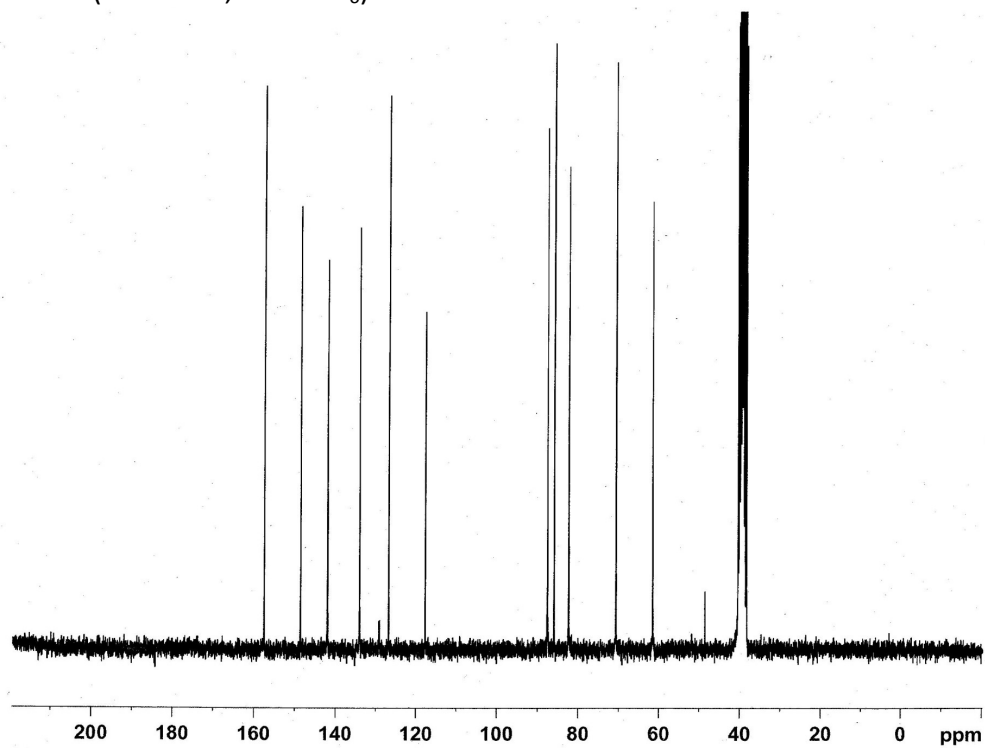


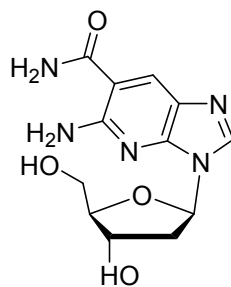
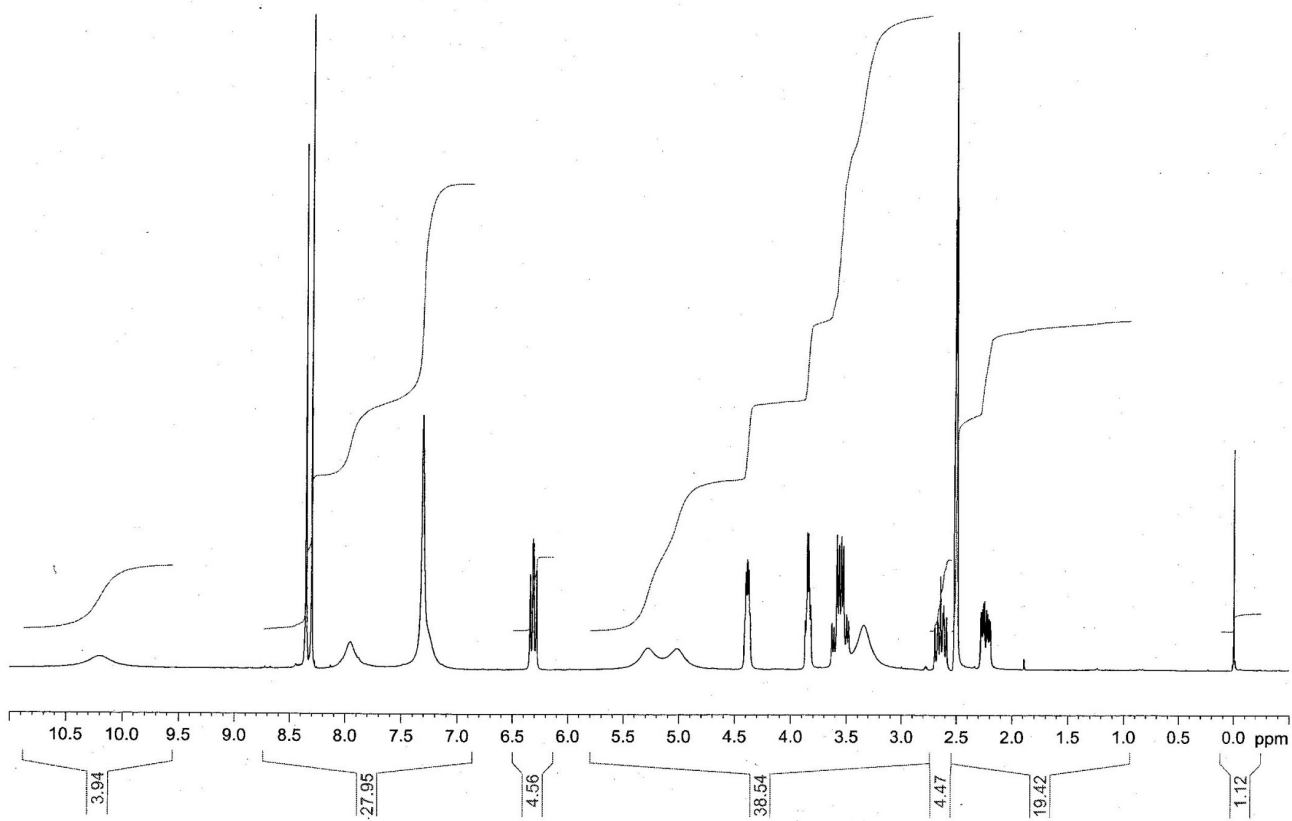
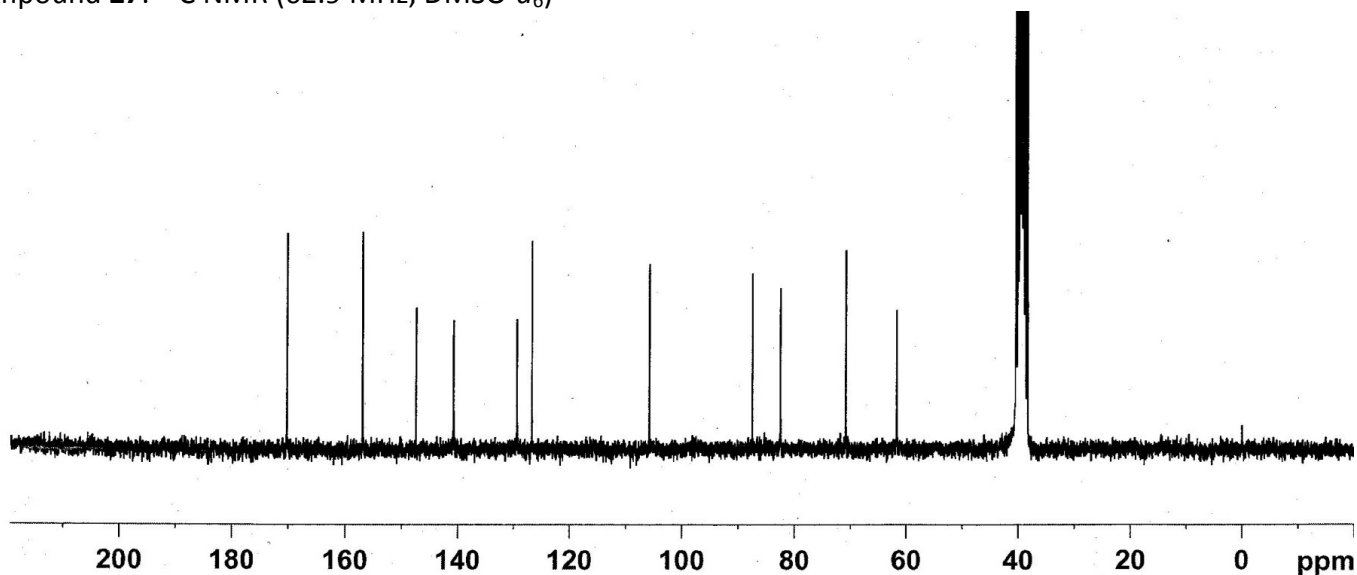
Compound **22**: <sup>13</sup>C NMR (62.9 MHz, DMSO-*d*<sub>6</sub>)

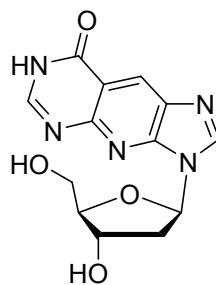


**23**Compound **23**: <sup>1</sup>H NMR (400.1 MHz, CDCl<sub>3</sub>)Compound **23**: <sup>13</sup>C NMR (101.6 MHz, CDCl<sub>3</sub>)

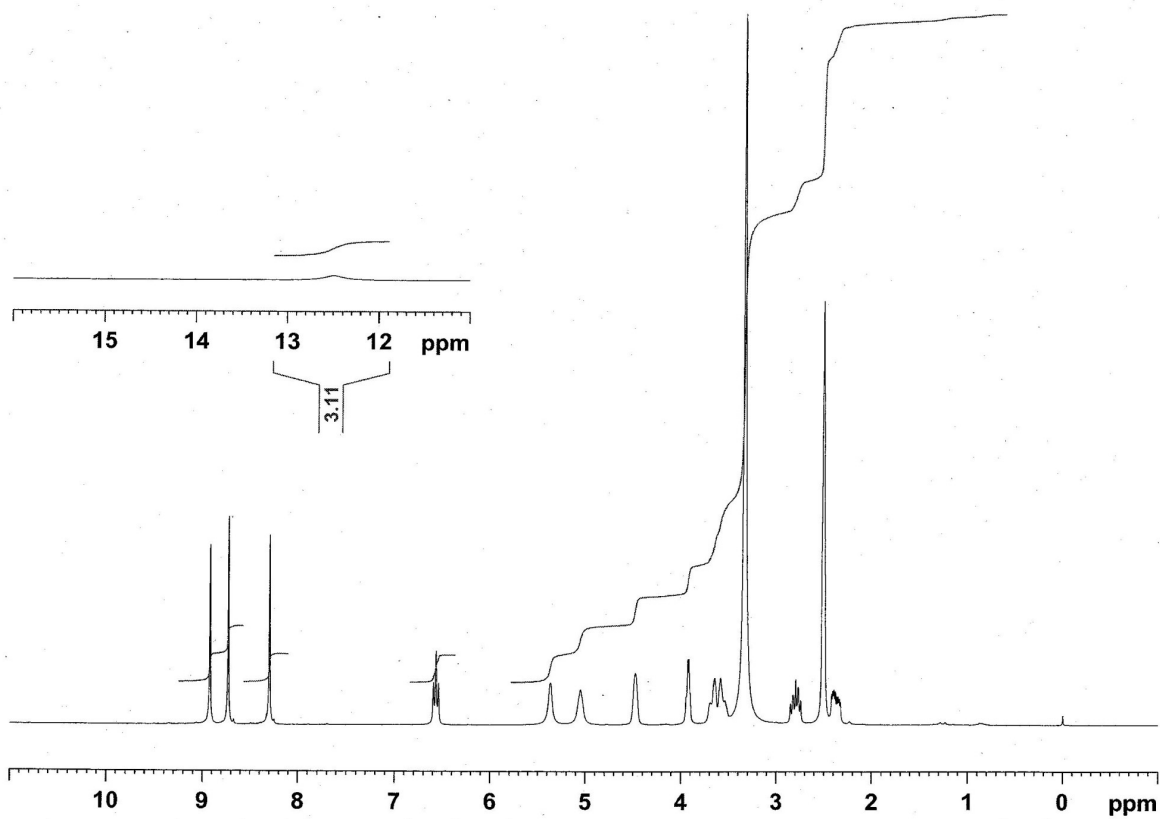
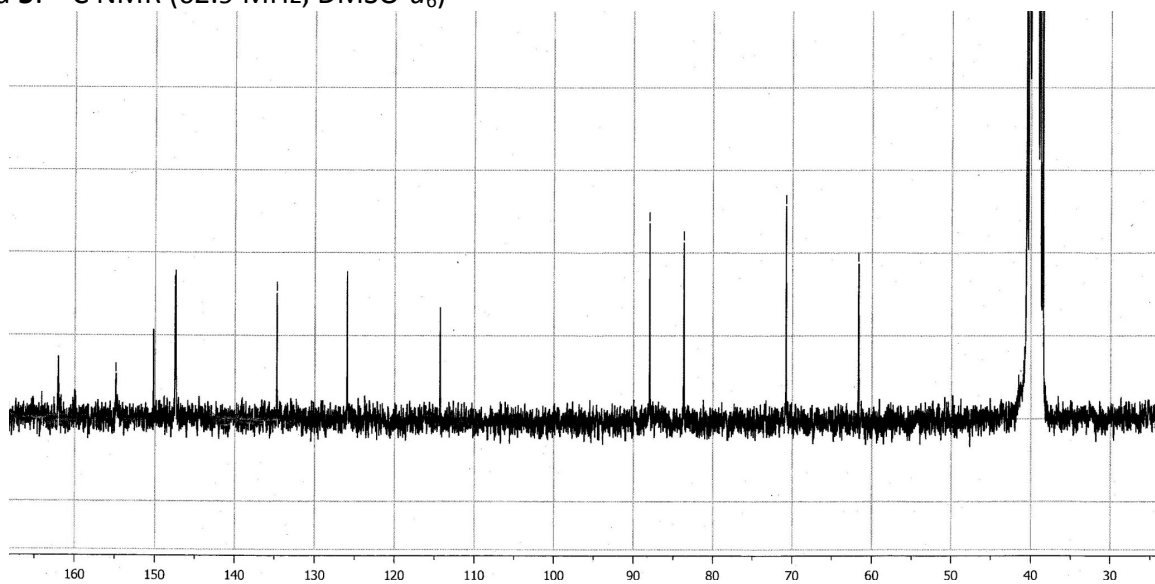
**26**Compound **26**: <sup>1</sup>H NMR (400.1 MHz, CDCl<sub>3</sub>)Compound **26**: <sup>13</sup>C NMR (101.6 MHz, CDCl<sub>3</sub>)

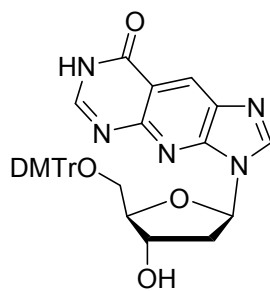
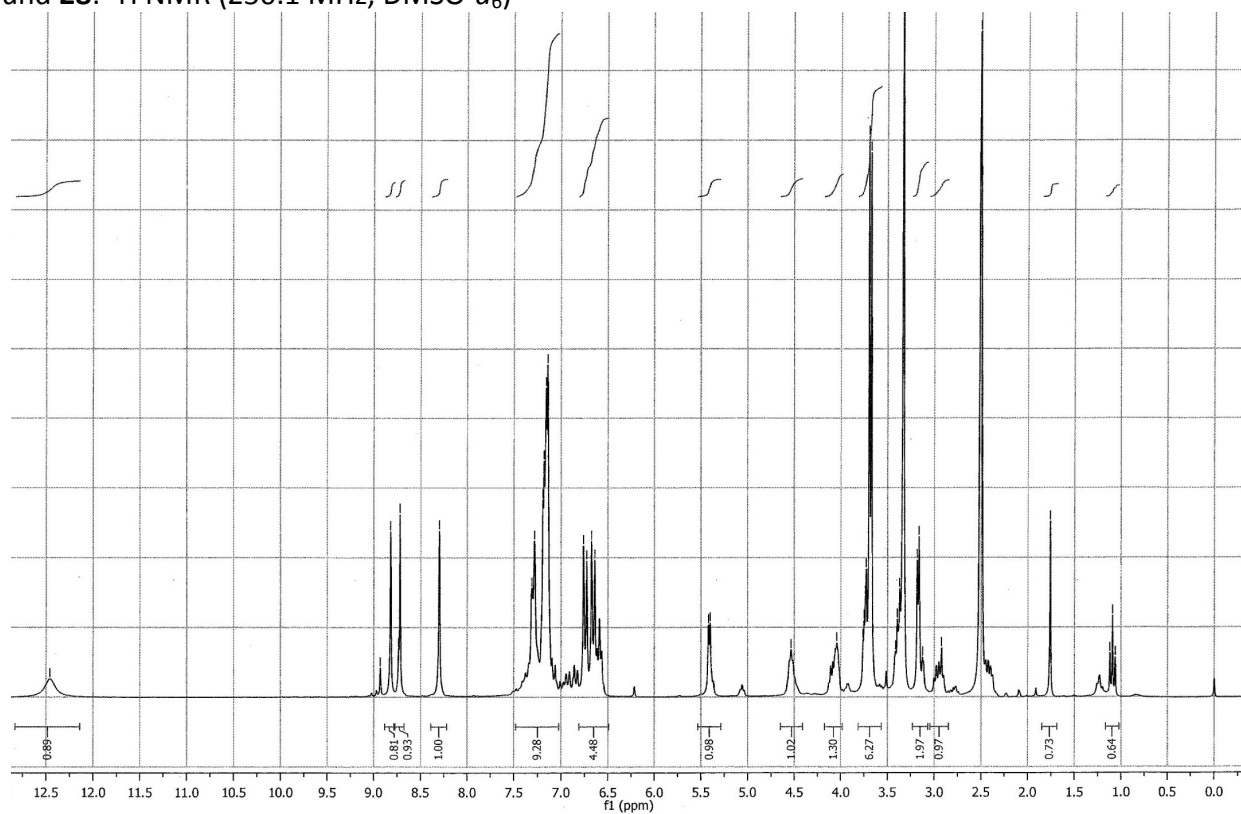
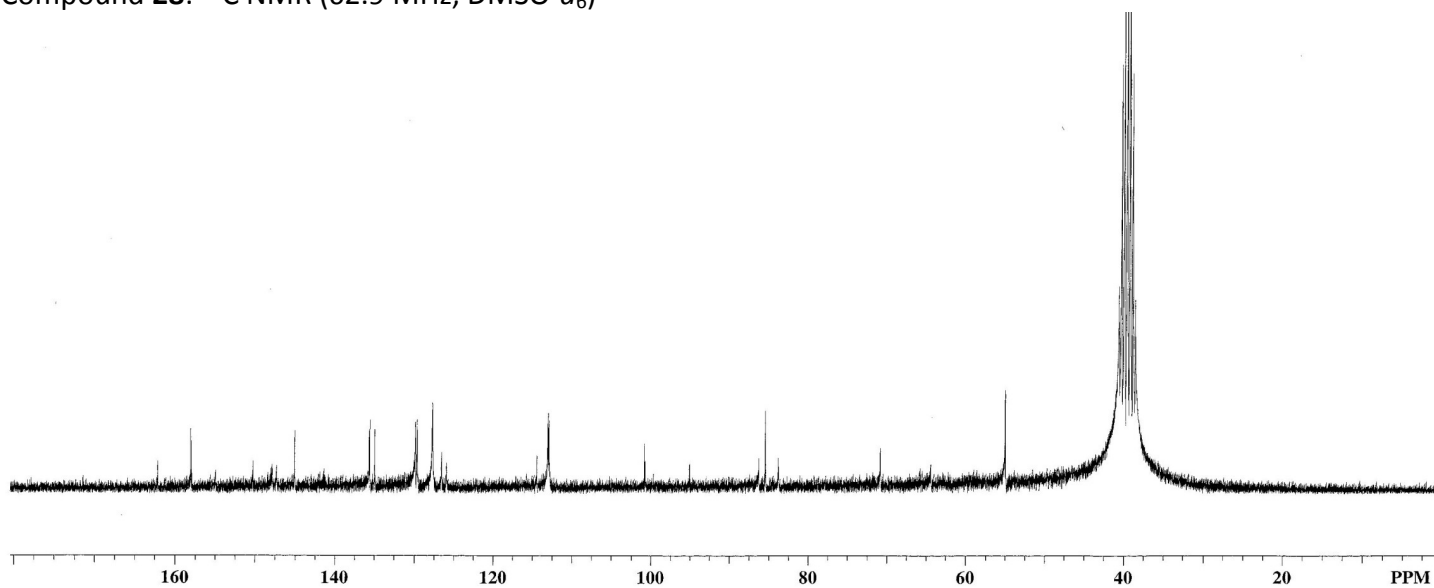
**24**Compound **24**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{DMSO-}d_6$ )Compound **24**:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{DMSO-}d_6$ )

**27**Compound **27**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{DMSO-}d_6$ )Compound **27**:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{DMSO-}d_6$ )

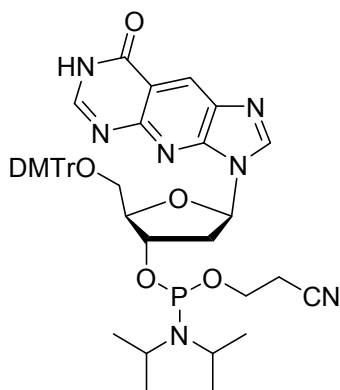
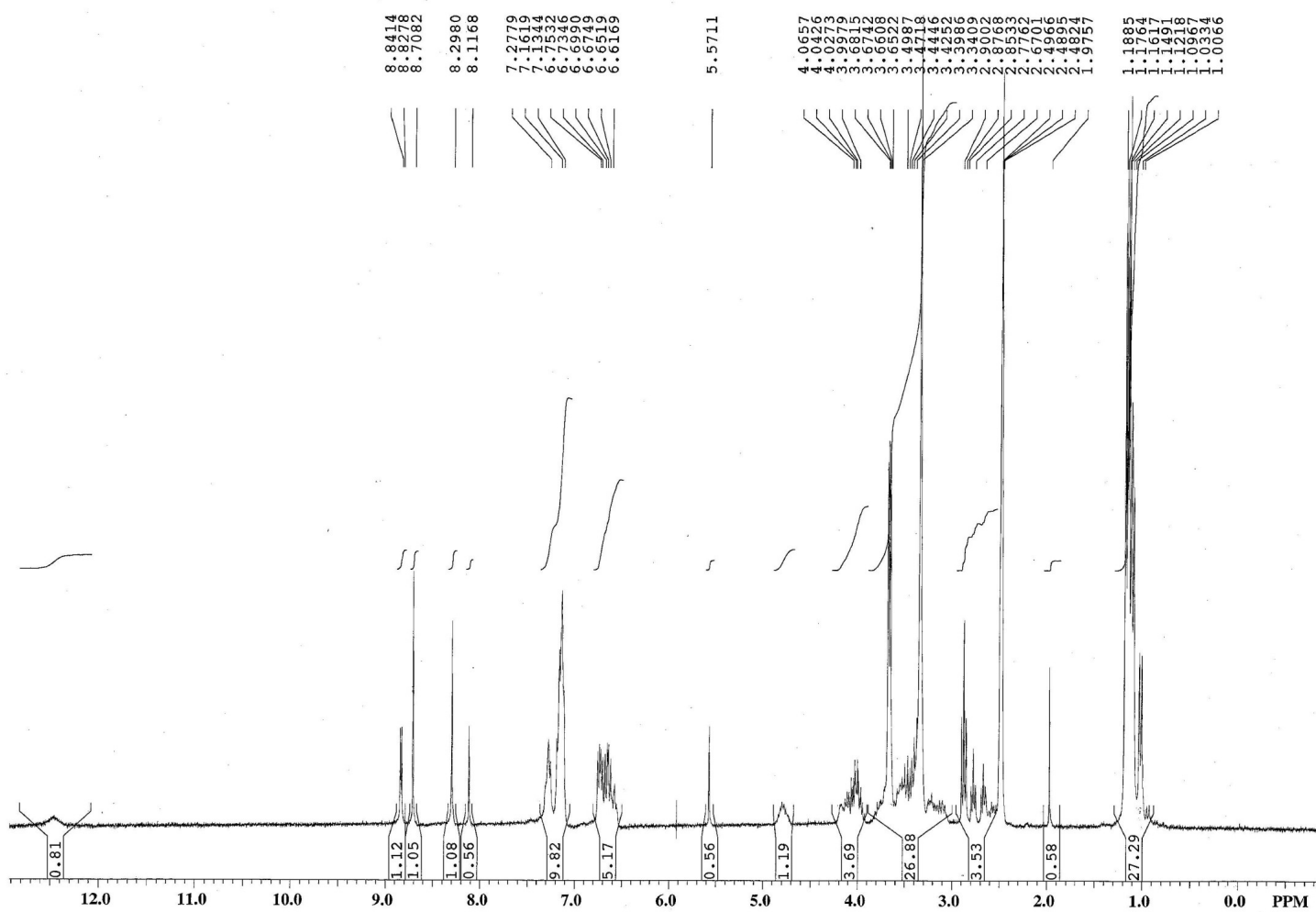


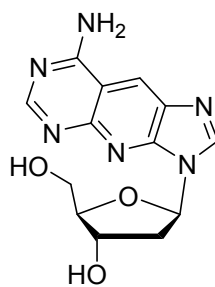
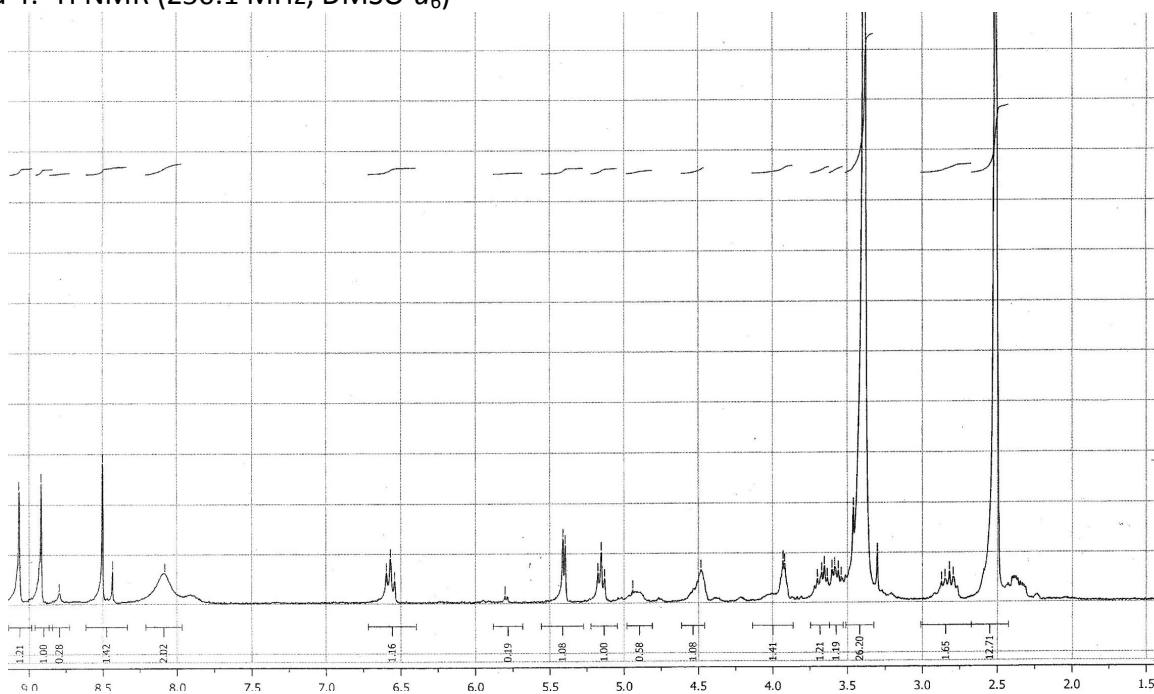
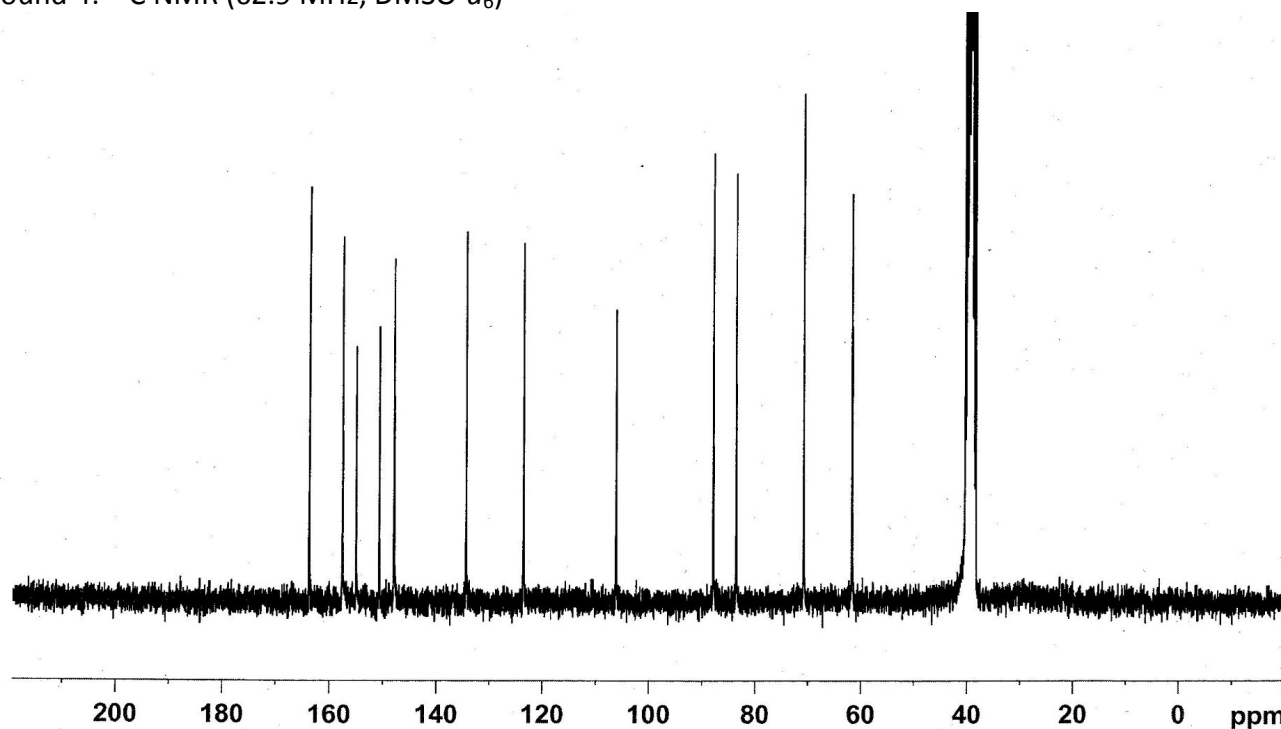
5

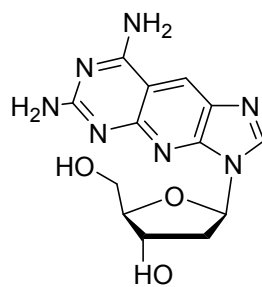
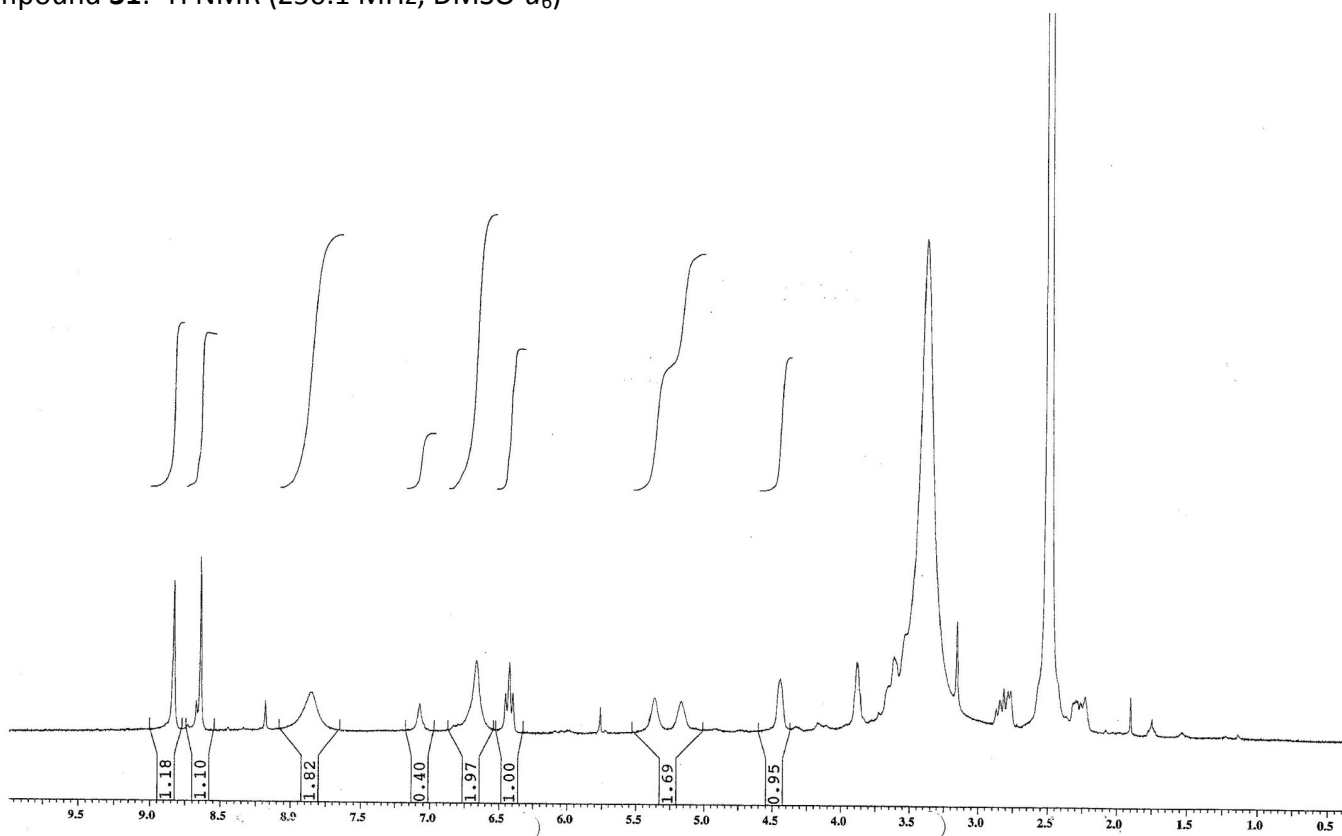
Compound 5:  $^1\text{H}$  NMR (250.1 MHz,  $\text{DMSO-}d_6$ )Compound 5:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{DMSO-}d_6$ )

**28**Compound **28**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{DMSO-}d_6$ )Compound **28**:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{DMSO-}d_6$ )



**30**Compound **30**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{DMSO-}d_6$ )

**4**Compound 4:  $^1\text{H}$  NMR (250.1 MHz,  $\text{DMSO-}d_6$ )Compound 4:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{DMSO-}d_6$ )

**31**Compound **31**:  $^1\text{H}$  NMR (250.1 MHz,  $\text{DMSO-}d_6$ )Compound **31**:  $^{13}\text{C}$  NMR (62.9 MHz,  $\text{DMSO-}d_6$ )