

Supplementary Material

A concise synthesis of isoguanine 2'-deoxyriboside and its adenine-like triplex formation when incorporated into DNA

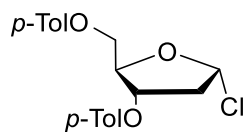
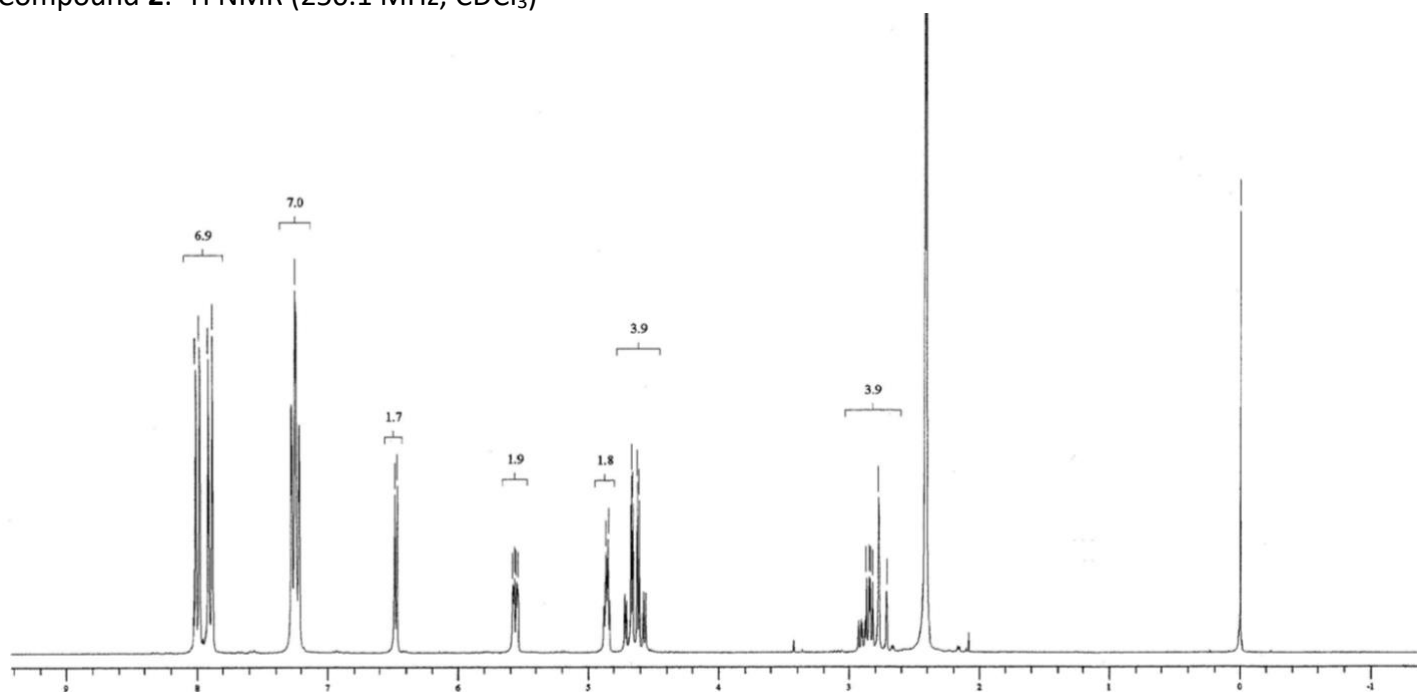
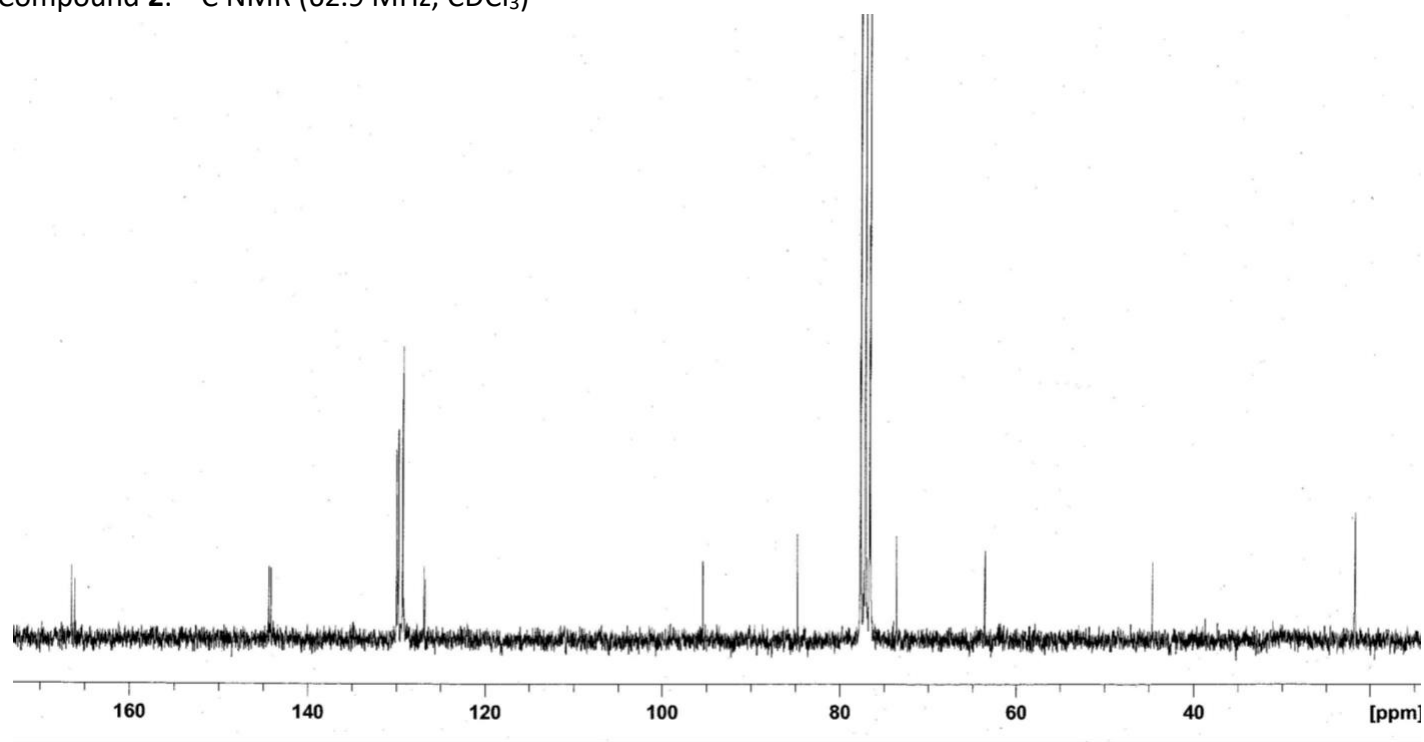
Andrew J. Walsh, Carl H. Schwalbe and William Fraser*

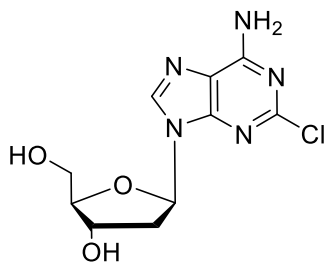
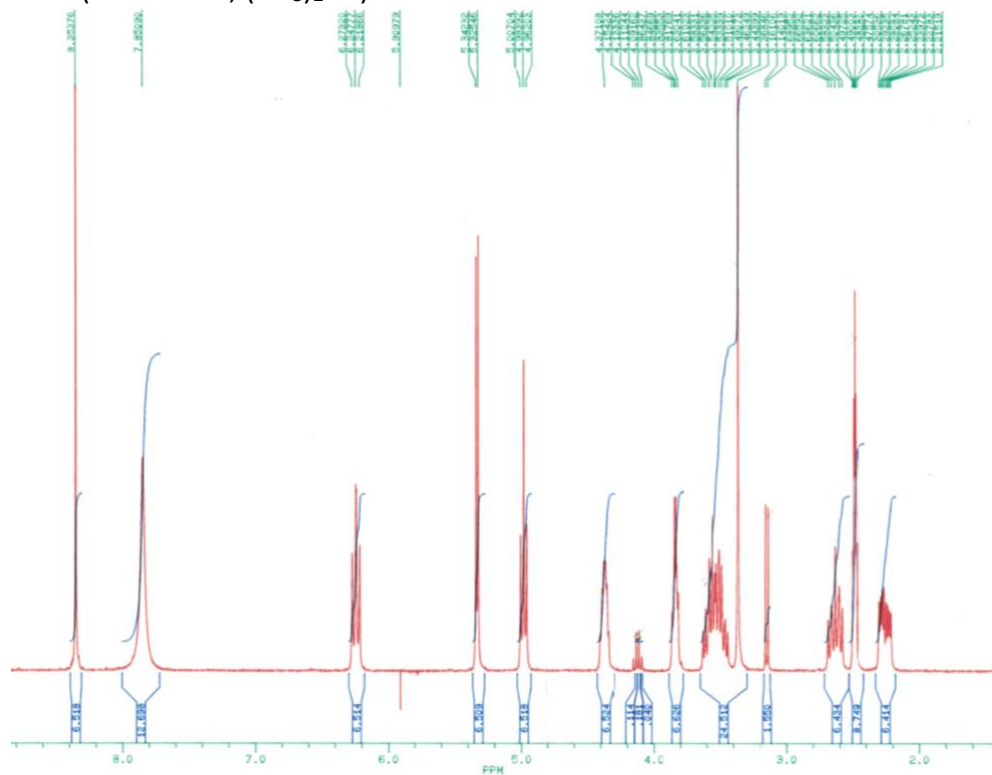
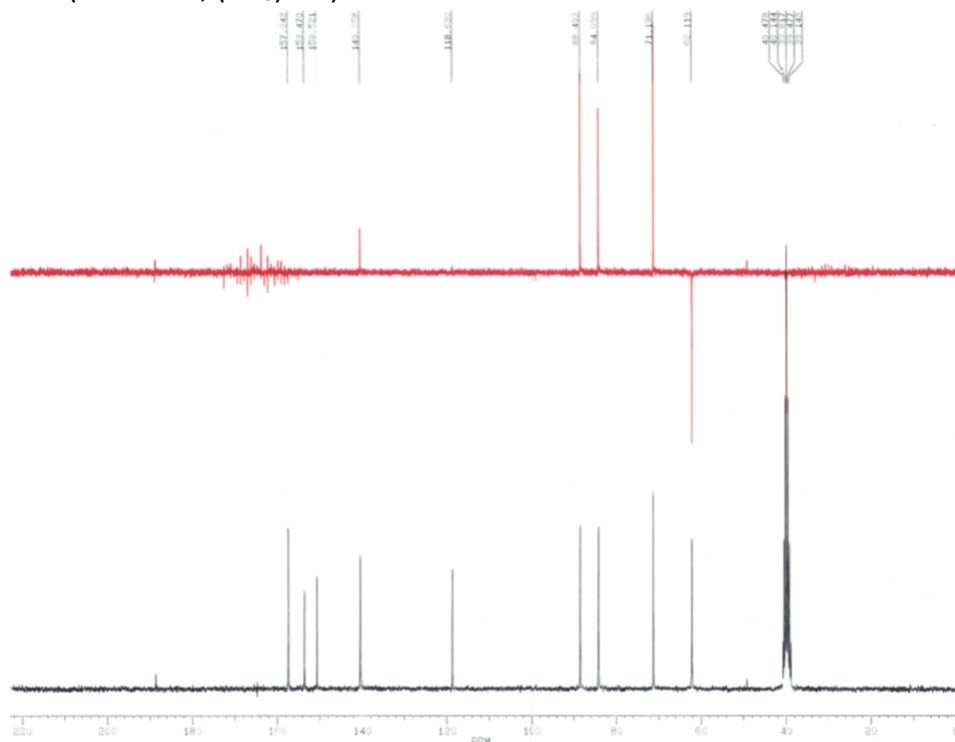
College of Health and Life Sciences, Aston University, Aston Triangle, Birmingham, B4 7ET, UK

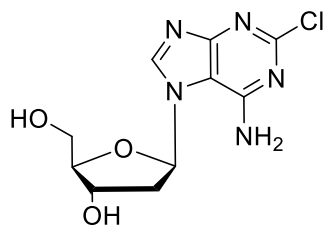
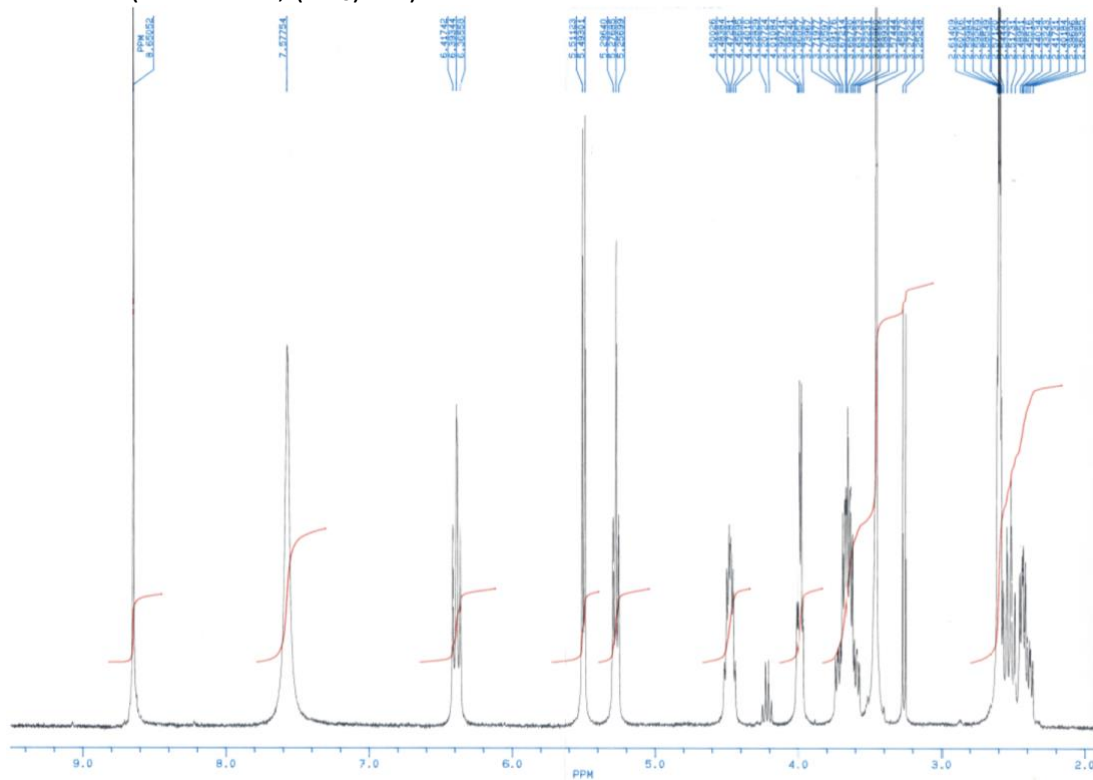
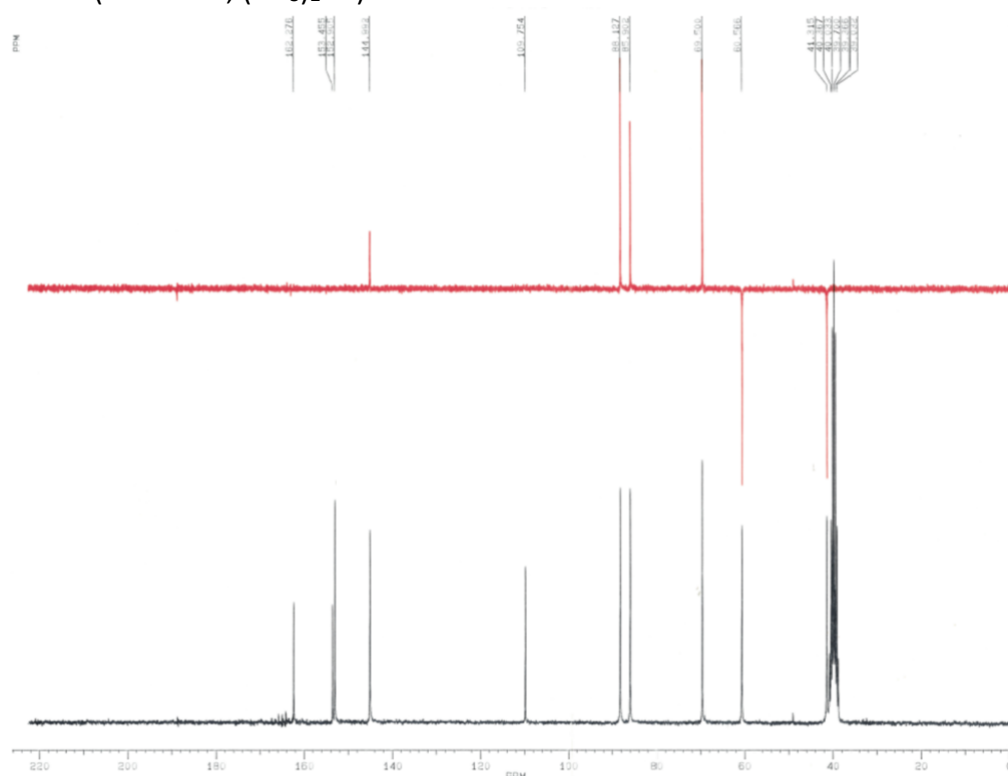
Email: w.fraser@aston.ac.uk

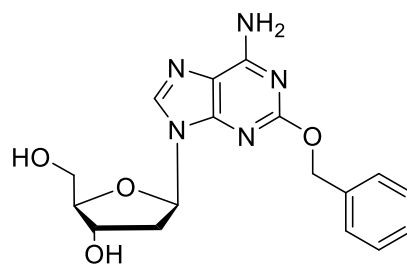
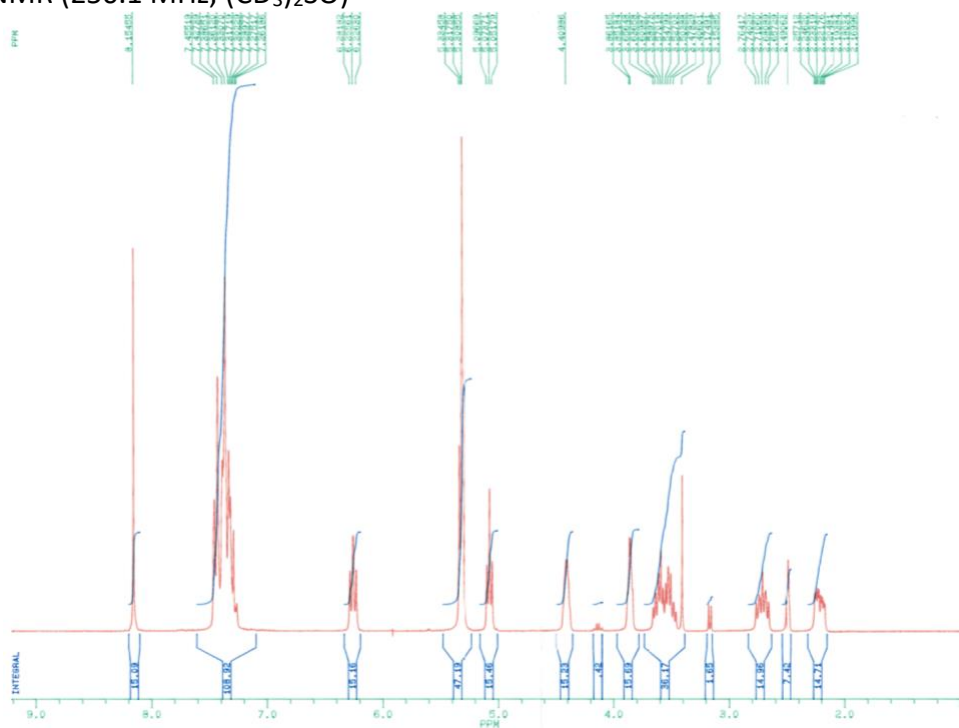
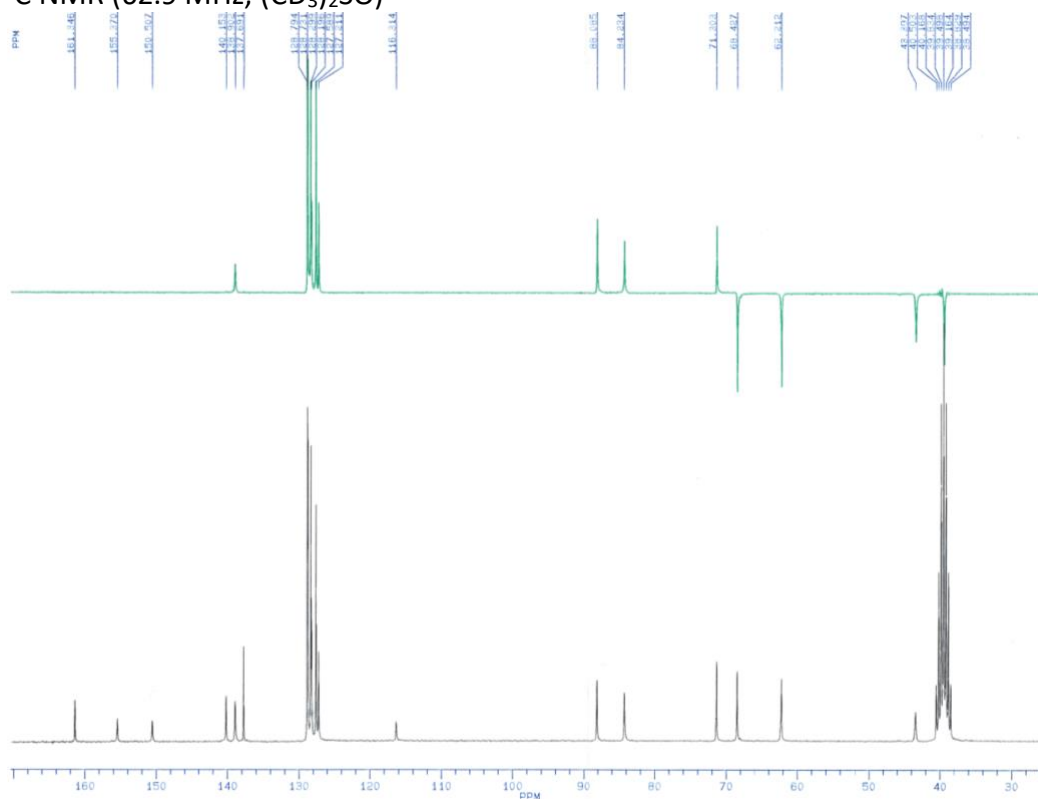
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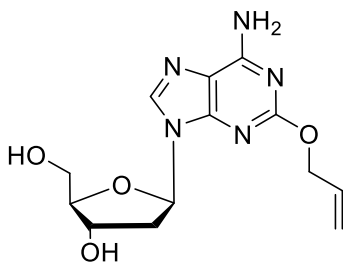
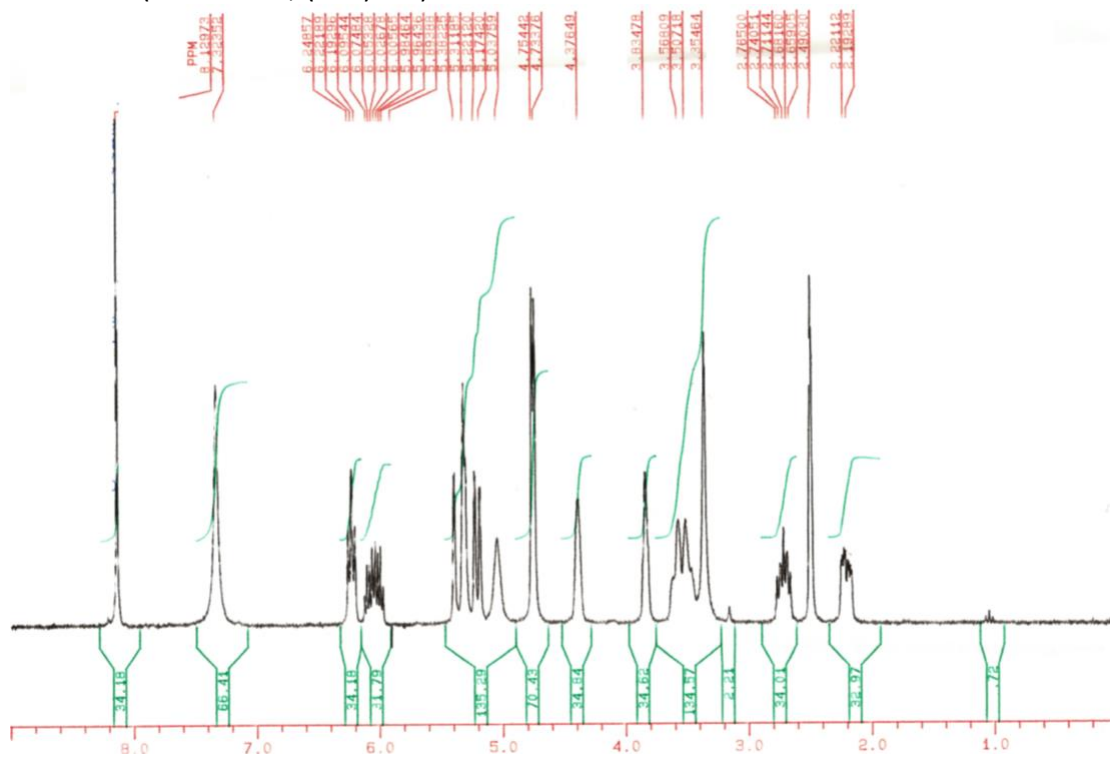
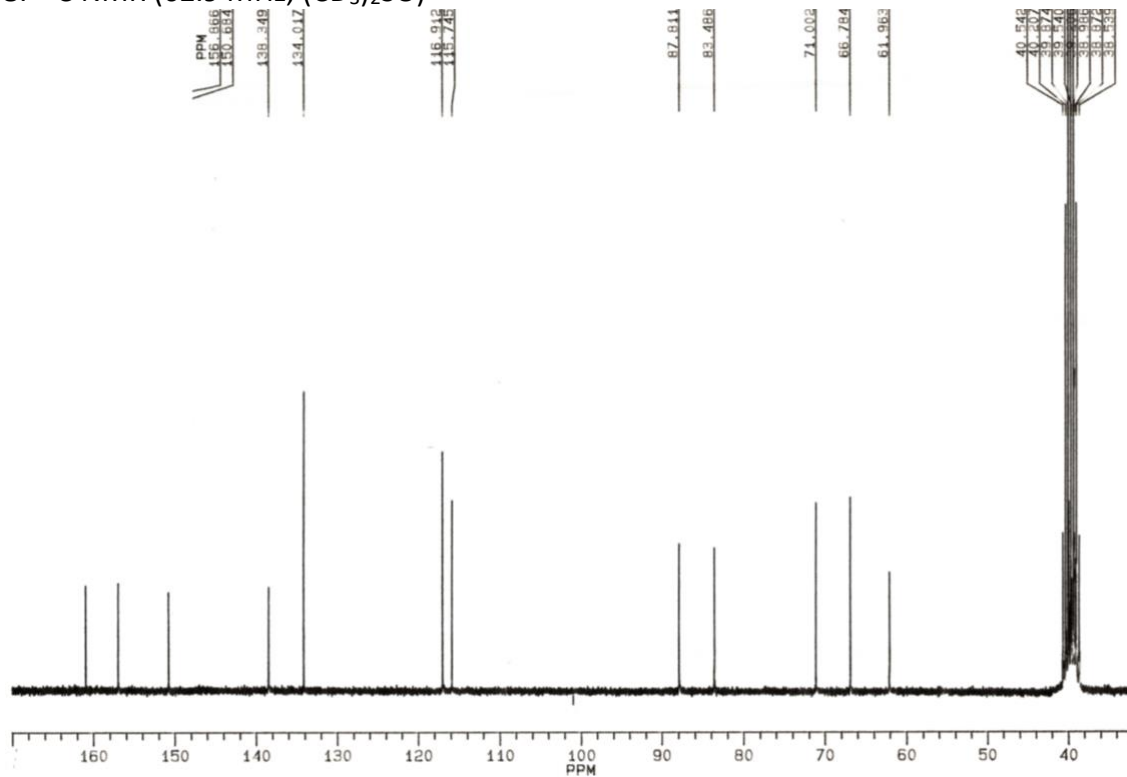
Compound 2 : ^1H NMR (250.1 MHz, CDCl_3)	S2
Compound 2 : ^{13}C NMR (62.9 MHz, CDCl_3)	S2
Compounds 3 and 4 : ^1H NMR (250.1 MHz, CDCl_3)	S3
Compound 5 : ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)	S4
Compound 5 : ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)	S4
Compound 6 : ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)	S5
Compound 6 : ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)	S5
Compound 7 : ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)	S6
Compound 7 : ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)	S6
Compound 8 : ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)	S7
Compound 8 : ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)	S7
Compound 9 : ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)	S8
Compound 9 : ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)	S8
Compound 11 : ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)	S9
Compound 11 : ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)	S9
Compound 13 : ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)	S10
Compound 13 : ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)	S10
Compound 14 : ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)	S11
Compound 14 : ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)	S11
Compound 14 : ^{31}P NMR (101.3 MHz, $(\text{CD}_3)_2\text{SO}$)	S12
Compound 15 : ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)	S13
Compound 15 : ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)	S13
Compound 15 : ^{31}P NMR (101.3 MHz, $(\text{CD}_3)_2\text{SO}$)	S14

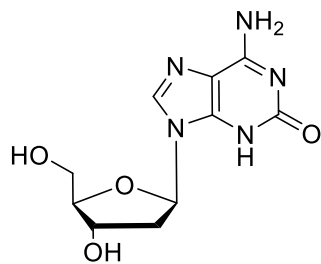
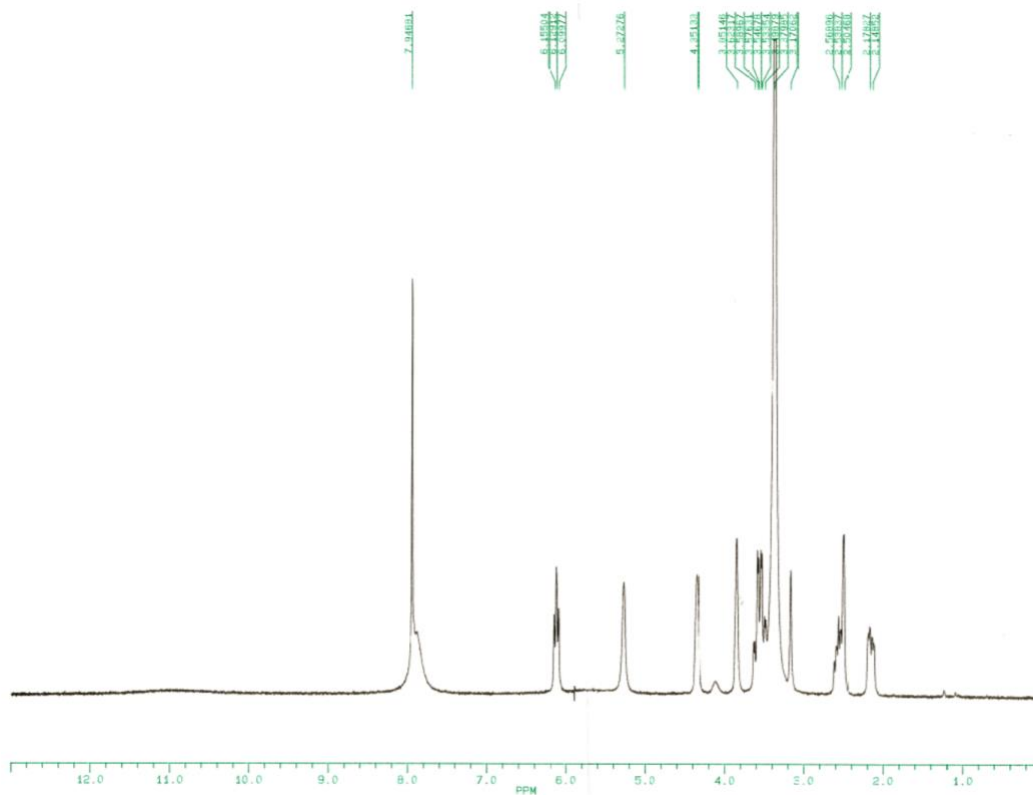
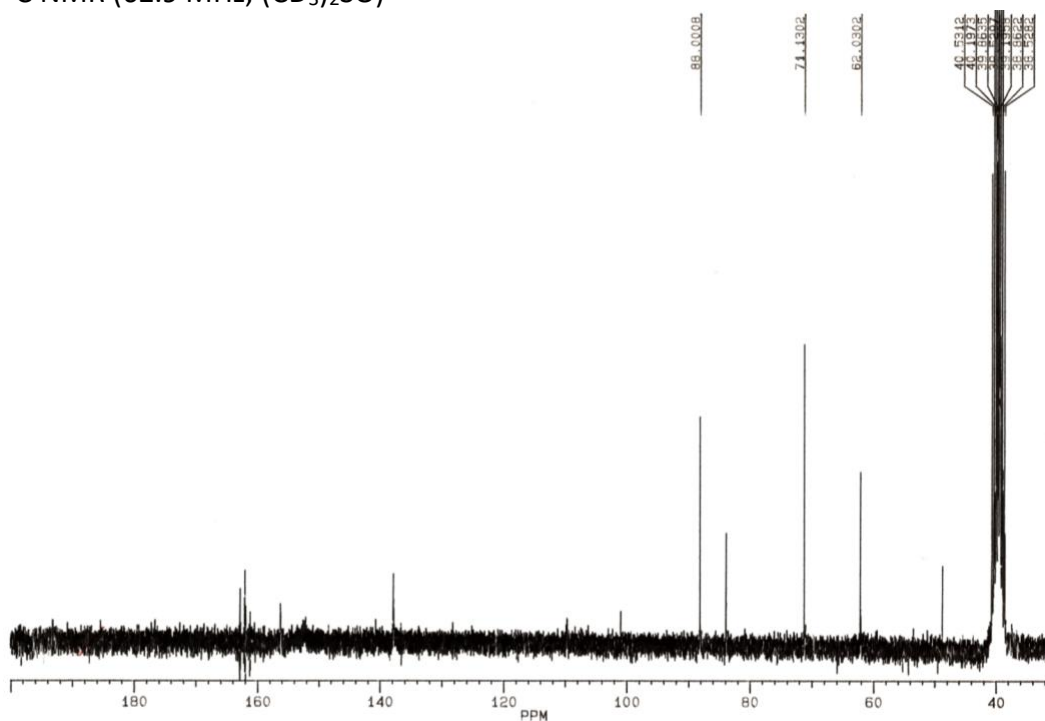
Compound **2**: ^1H NMR (250.1 MHz, CDCl_3)Compound **2**: ^{13}C NMR (62.9 MHz, CDCl_3)

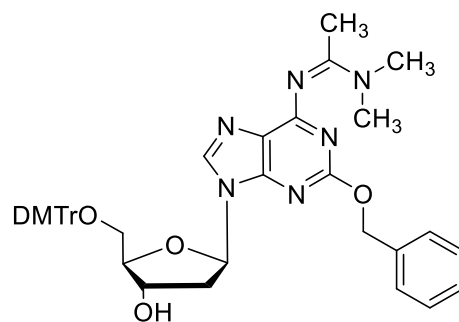
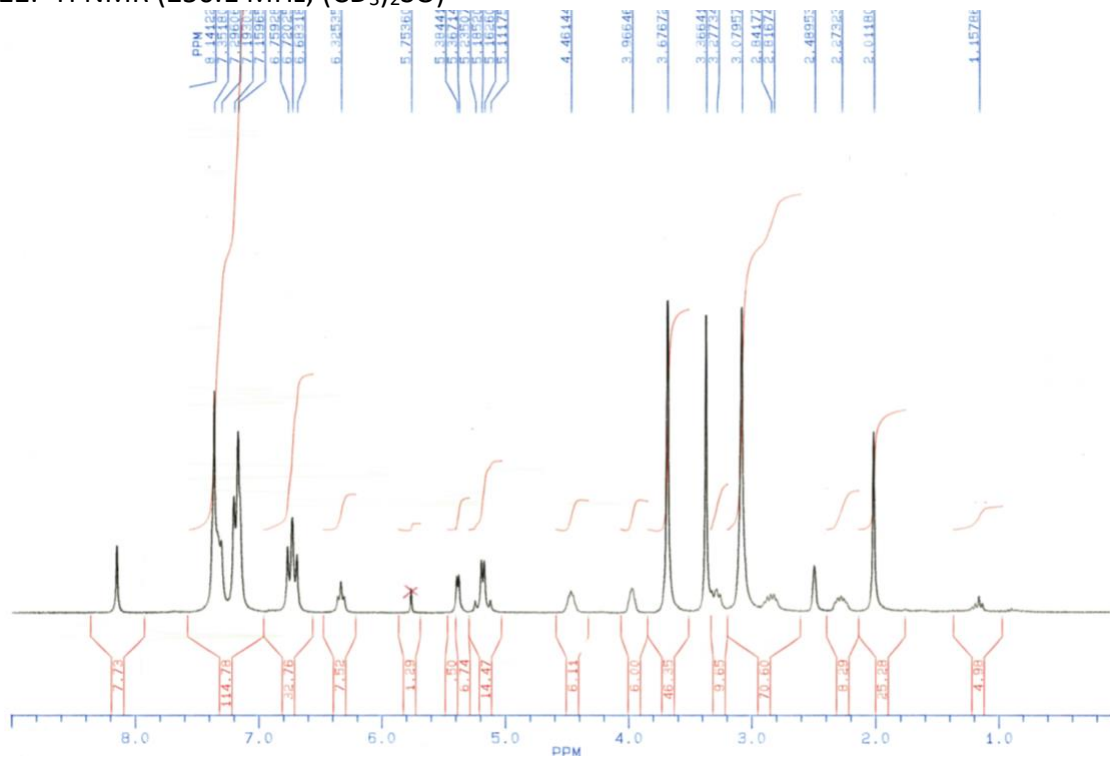
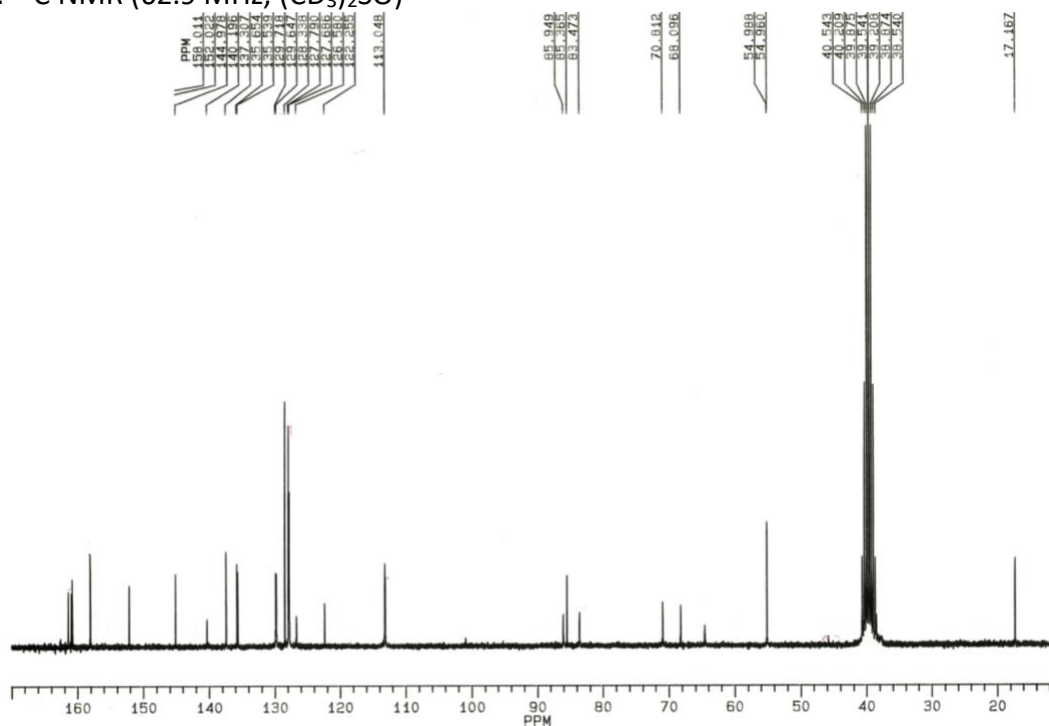
Compound 5: ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)Compound 5: ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)

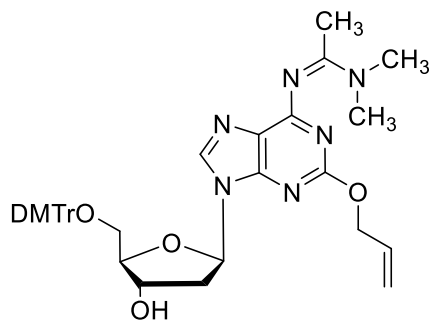
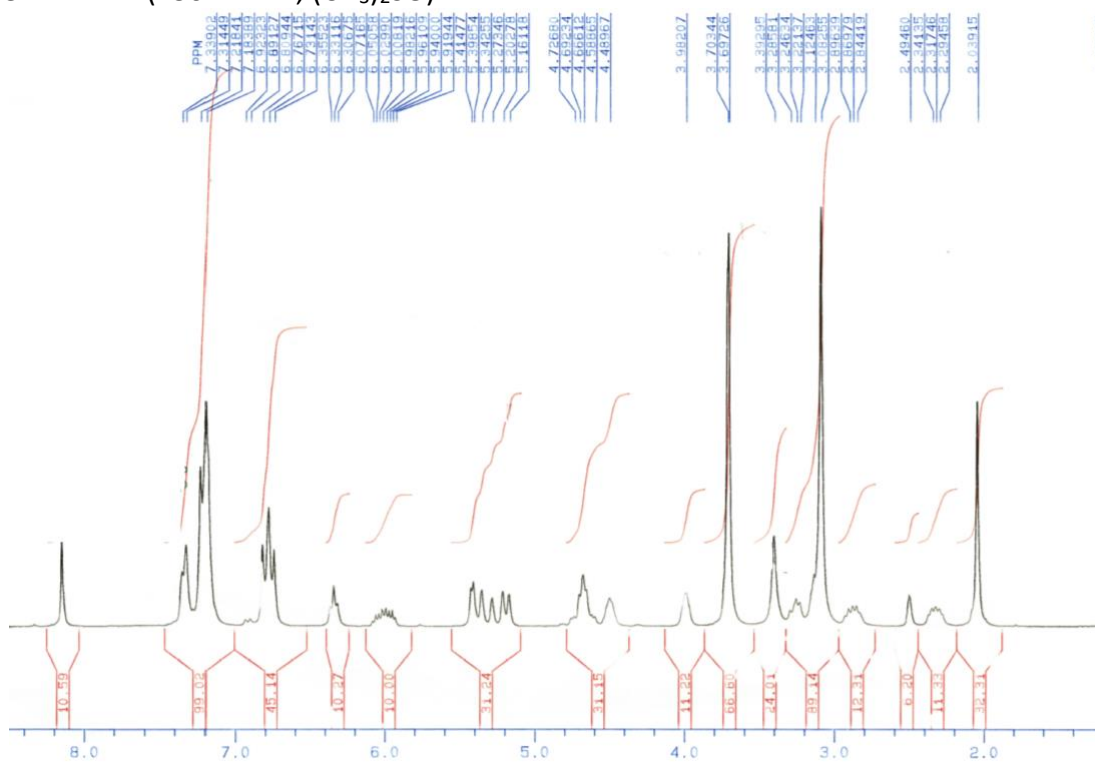
Compound 6: ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)Compound 6: ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)

Compound 7: ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)Compound 7: ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)

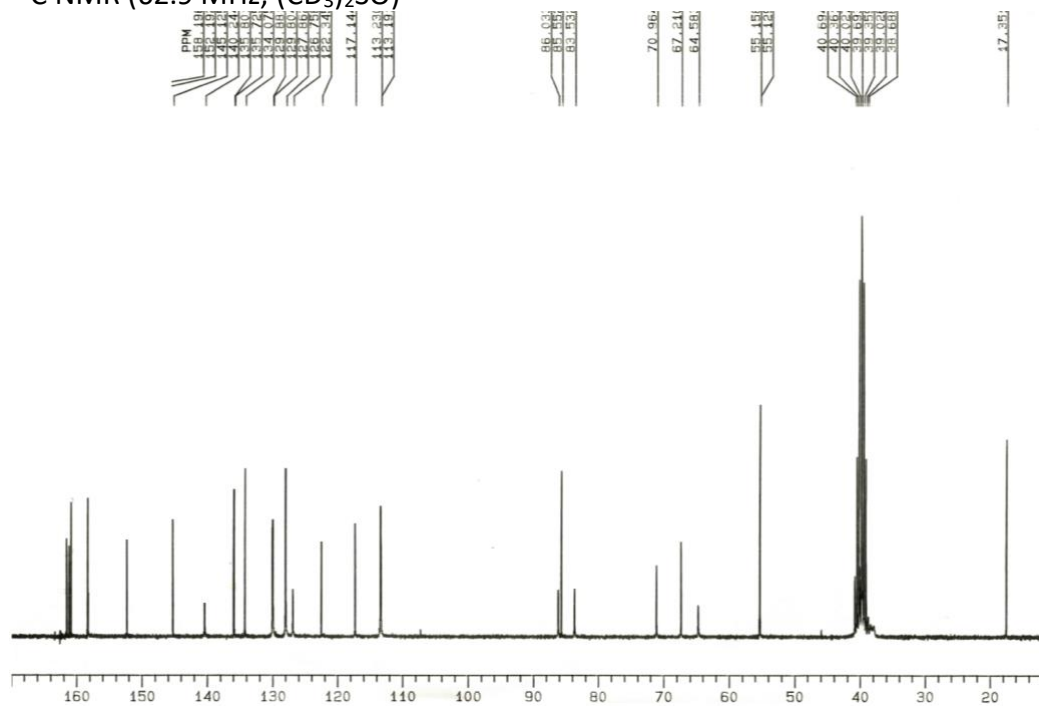
Compound **8**: ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)Compound **8**: ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)

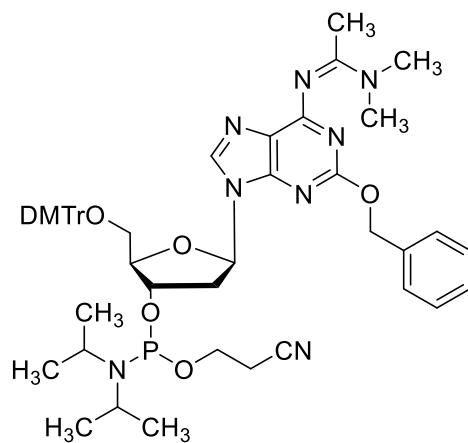
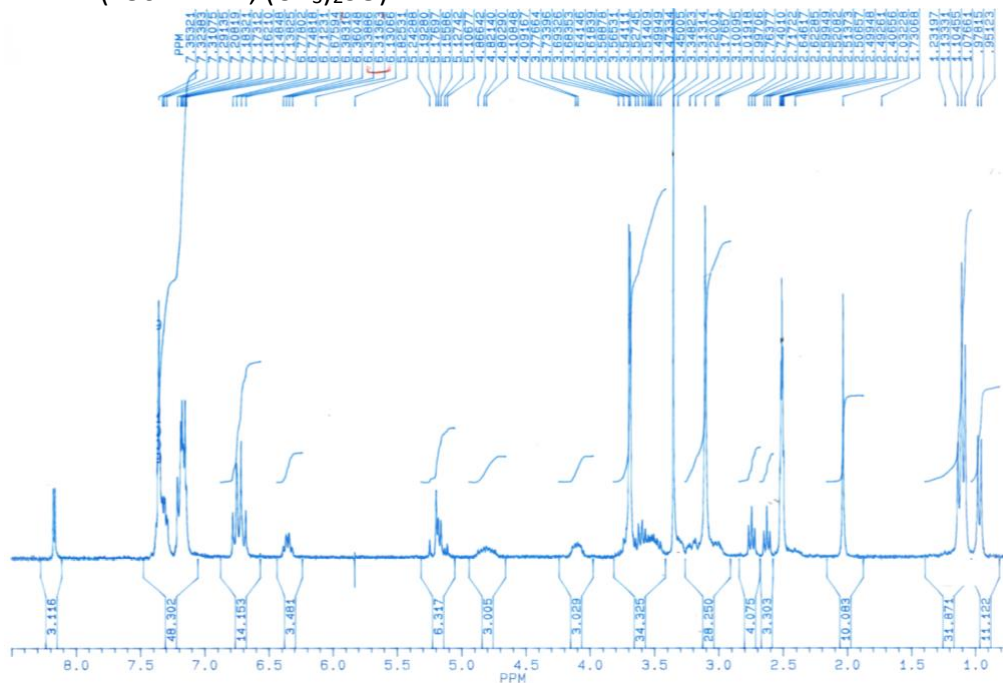
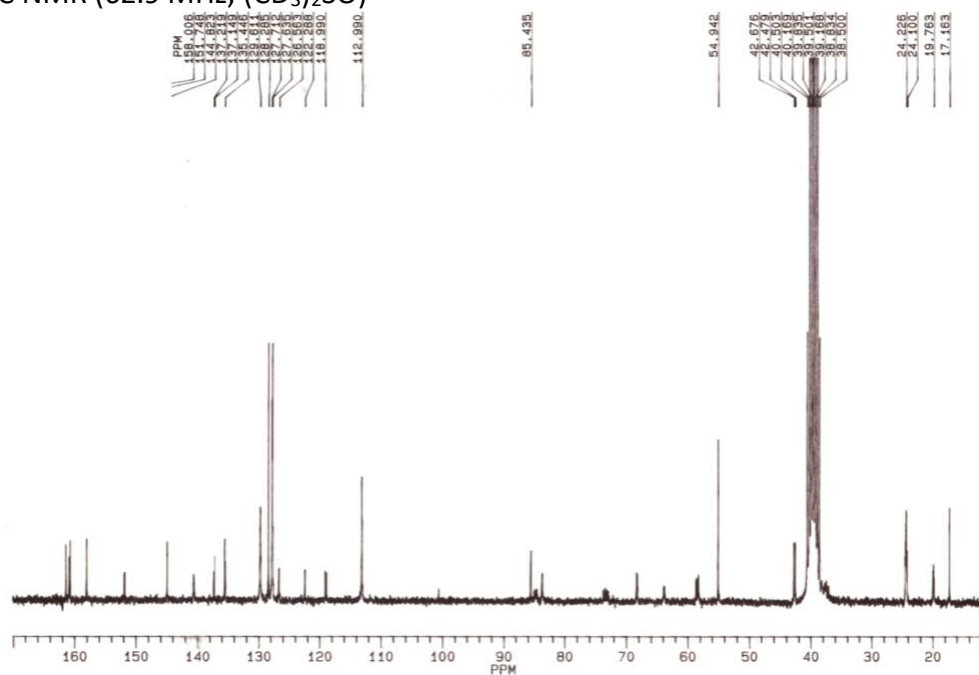
Compound **9**: ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)Compound **9**: ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)

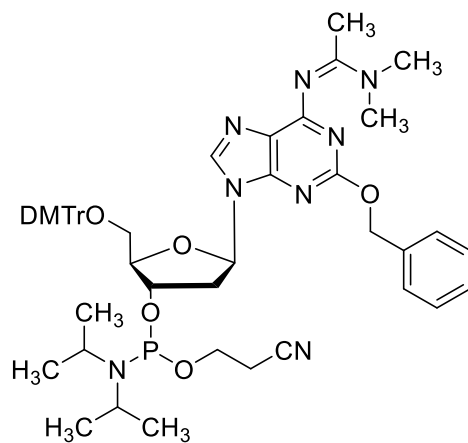
Compound 11: ¹H NMR (250.1 MHz, (CD₃)₂SO)Compound 11: ¹³C NMR (62.9 MHz, (CD₃)₂SO)

Compound **13**: ^1H NMR (250.1 MHz, $(\text{CD}_3)_2\text{SO}$)

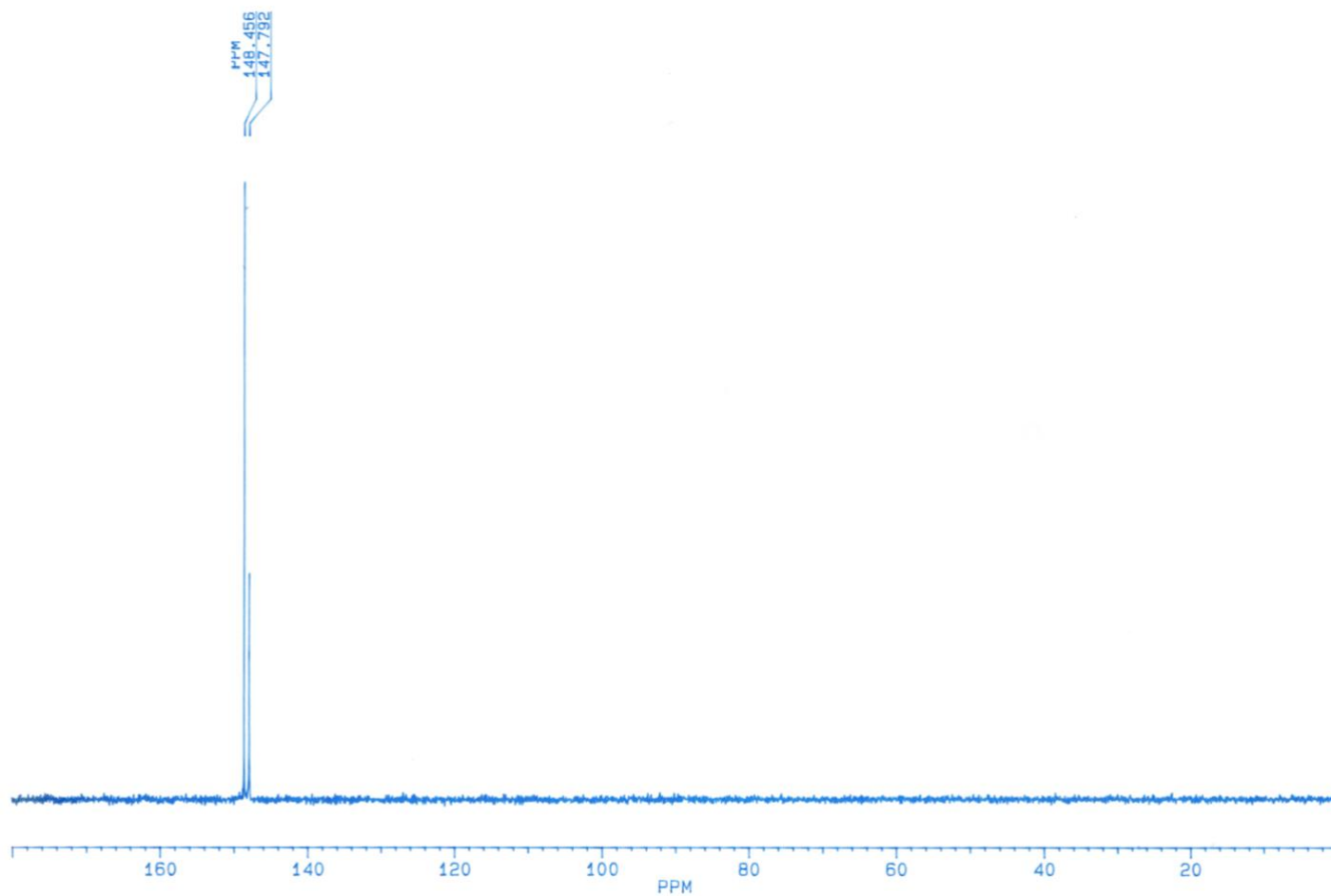
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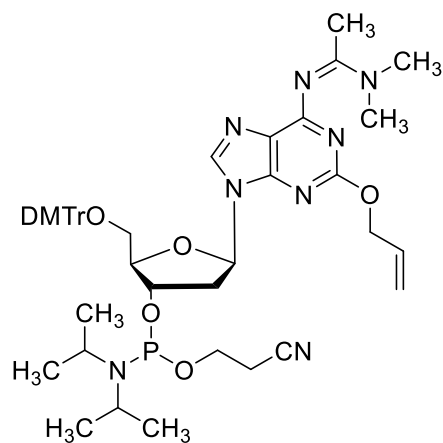
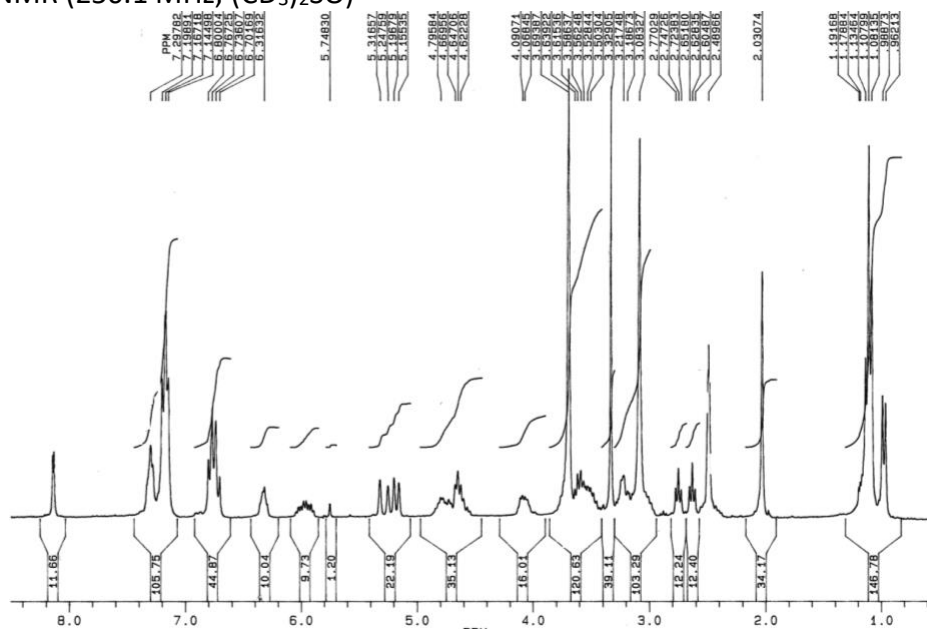
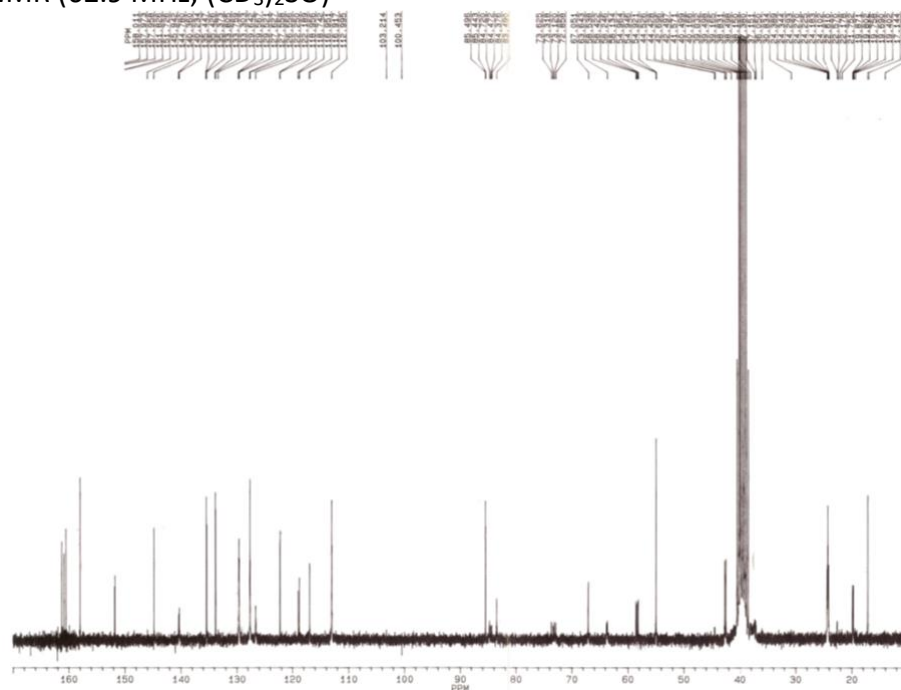
Compound **13**: ^{13}C NMR (62.9 MHz, $(\text{CD}_3)_2\text{SO}$)

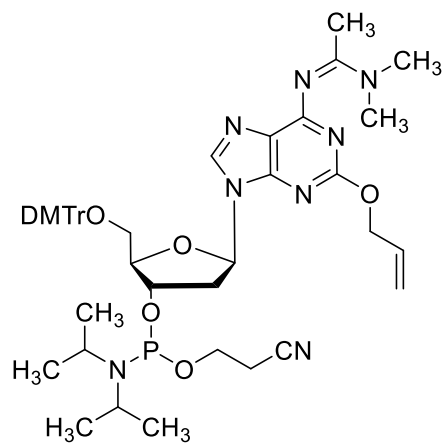
Compound 14: ¹H NMR (250.1 MHz, (CD₃)₂SO)Compound 14: ¹³C NMR (62.9 MHz, (CD₃)₂SO)



Compound **14**: ³¹P NMR (101.3 MHz, (CD₃)₂SO)



Compound 15: ¹H NMR (250.1 MHz, (CD₃)₂SO)Compound 15: ¹³C NMR (62.9 MHz, (CD₃)₂SO)

Compound **15**: ³¹P NMR (101.3 MHz, (CD₃)₂SO)