

Supporting Information

Synthesis of triazole-linked SAM-adenosine conjugates: functionalization of adenosine at N1 or N6 position without protecting groups

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Emmanuelle Braud*

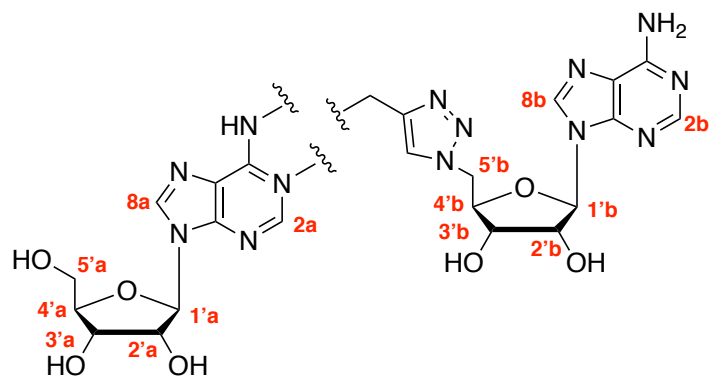
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Table of contents

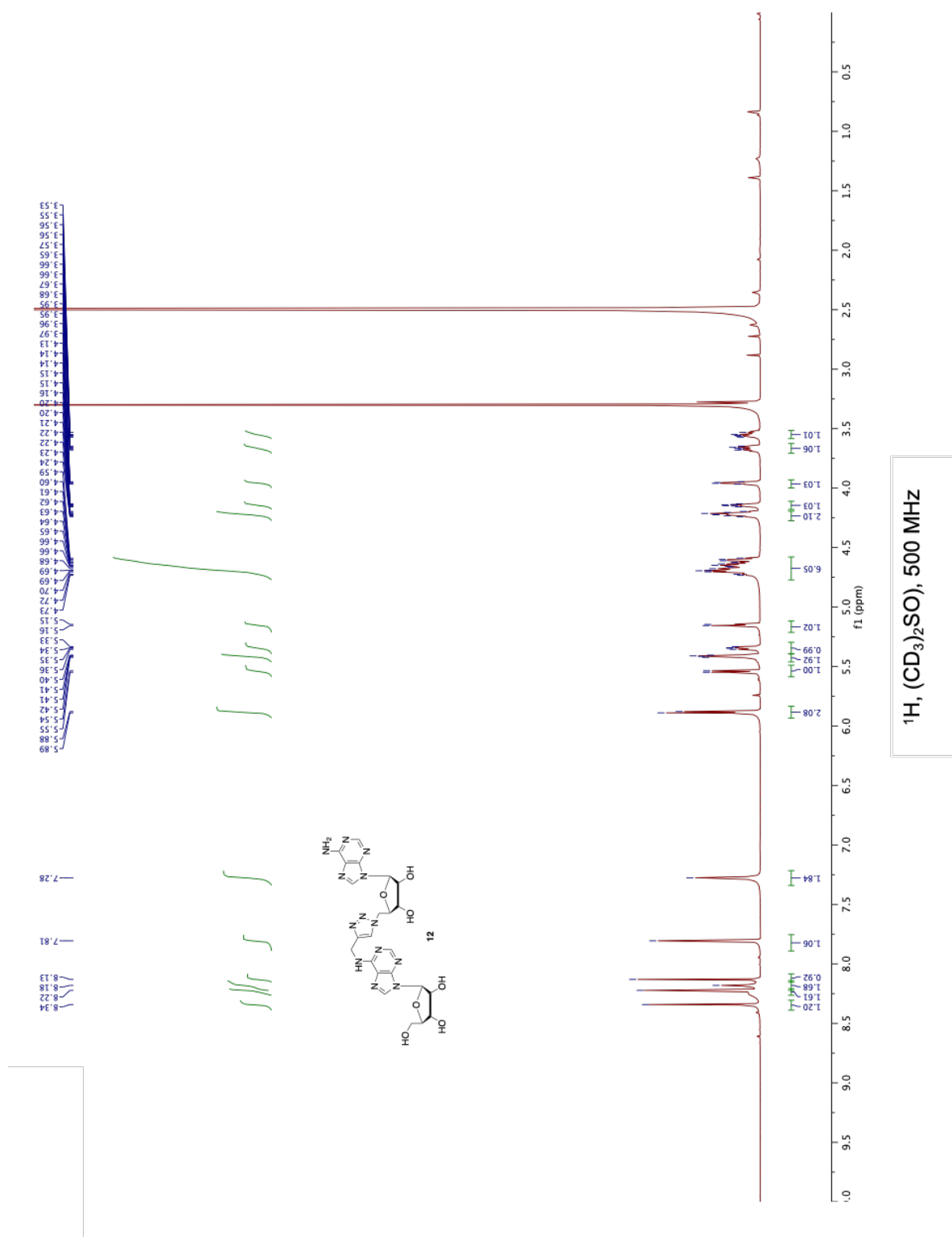
1. Numbering of synthesized molecules.....	S3
2. NMR spectra of final compounds	S4
Compound 12 (^1H and ^{13}C spectra).....	S4
Compound 13 (^1H and ^{13}C spectra).....	S6
Compound 14 (^1H and ^{13}C spectra).....	S8
Compound 15 (^1H and ^{13}C spectra).....	S10
Compound 19 (^1H and ^{13}C spectra).....	S12
3. HPLC spectra of final compounds	S14
HPLC trace of compound 12	S14
HPLC trace of compound 13	S14
HPLC trace of compound 14	S15
HPLC trace of compound 15	S15
HPLC trace of compound 19	S16

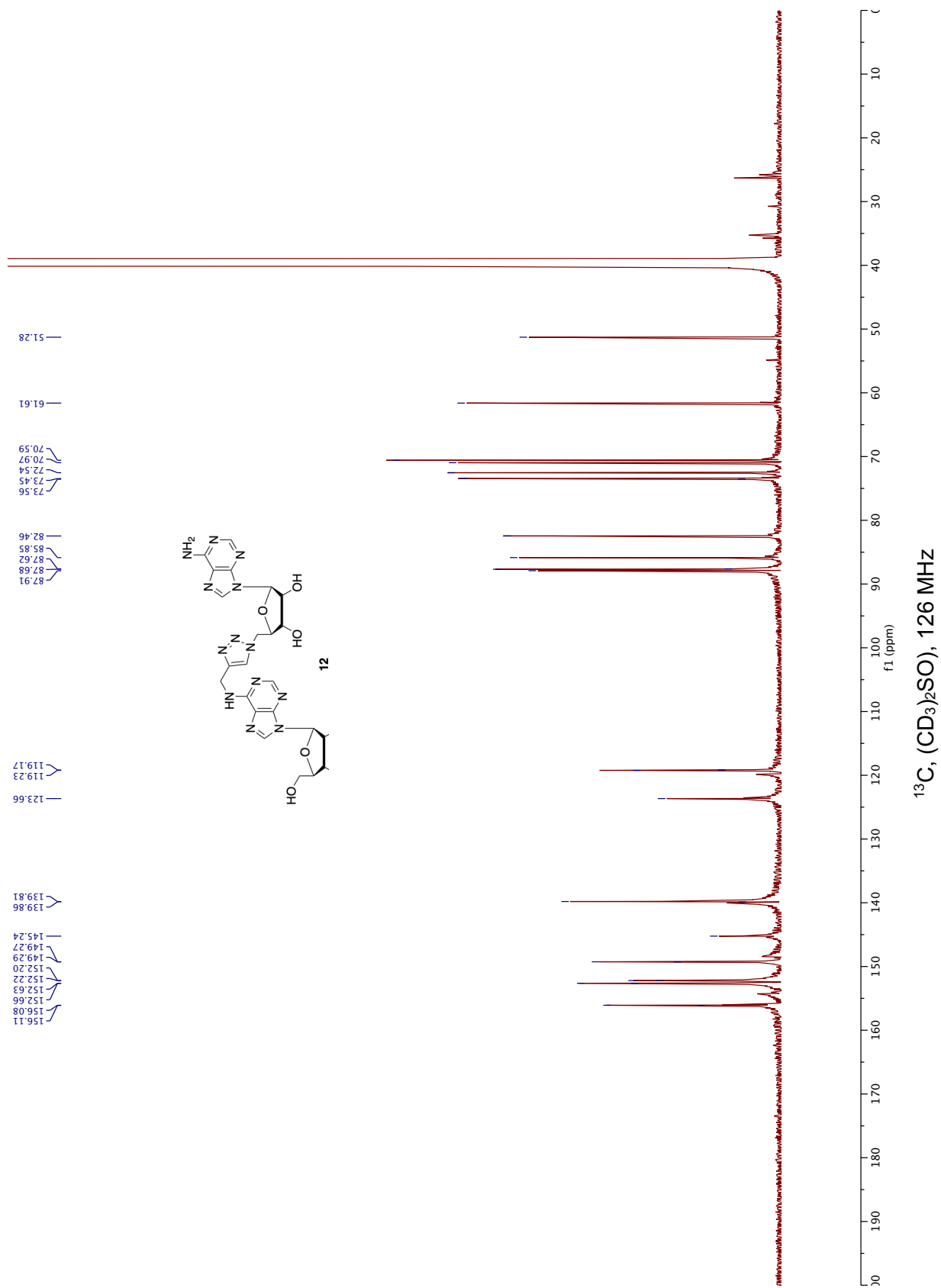
1. Numbering of synthesized molecules

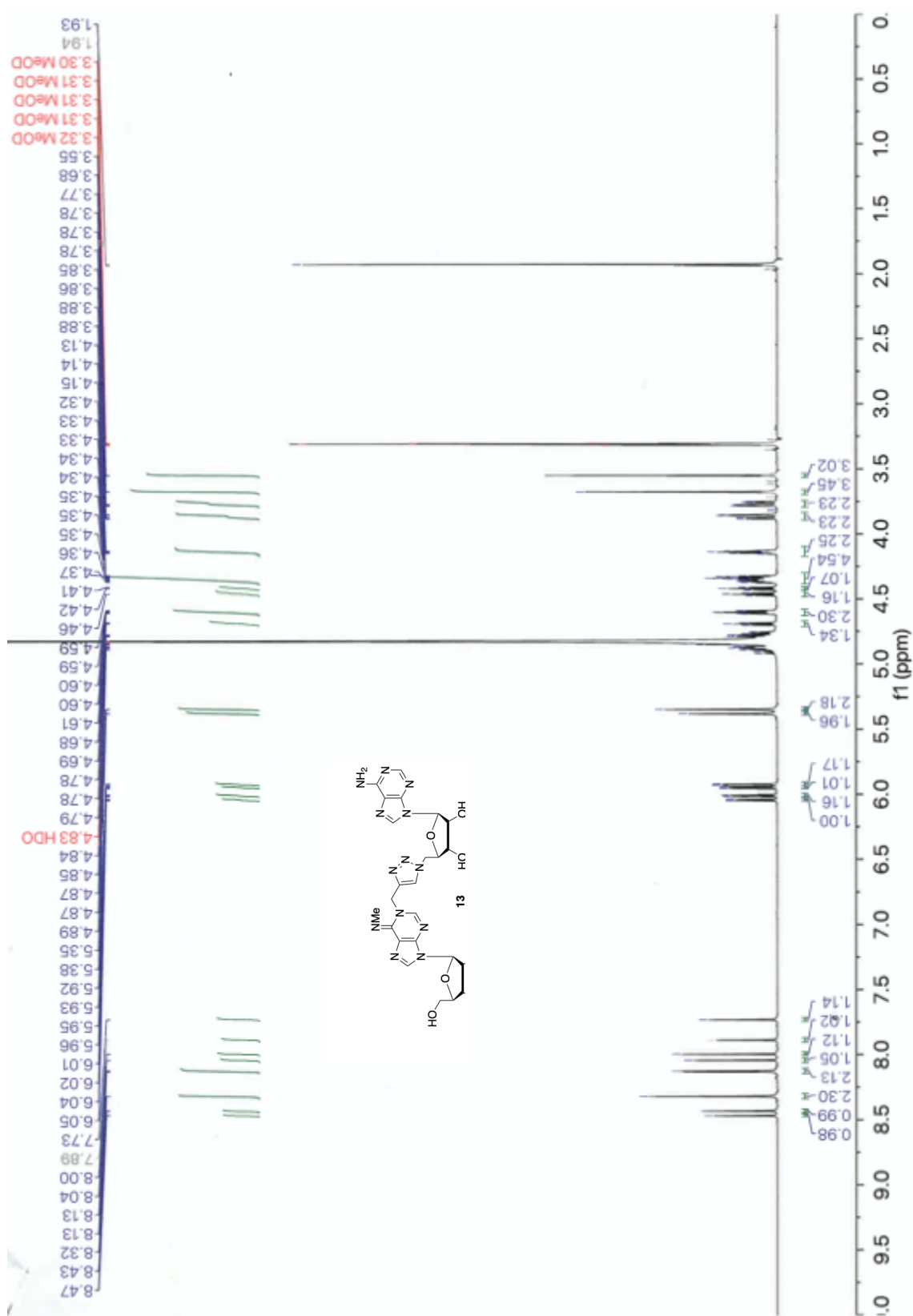
Characterizations of the synthesized compounds are indicated according to the following numbering of atoms:



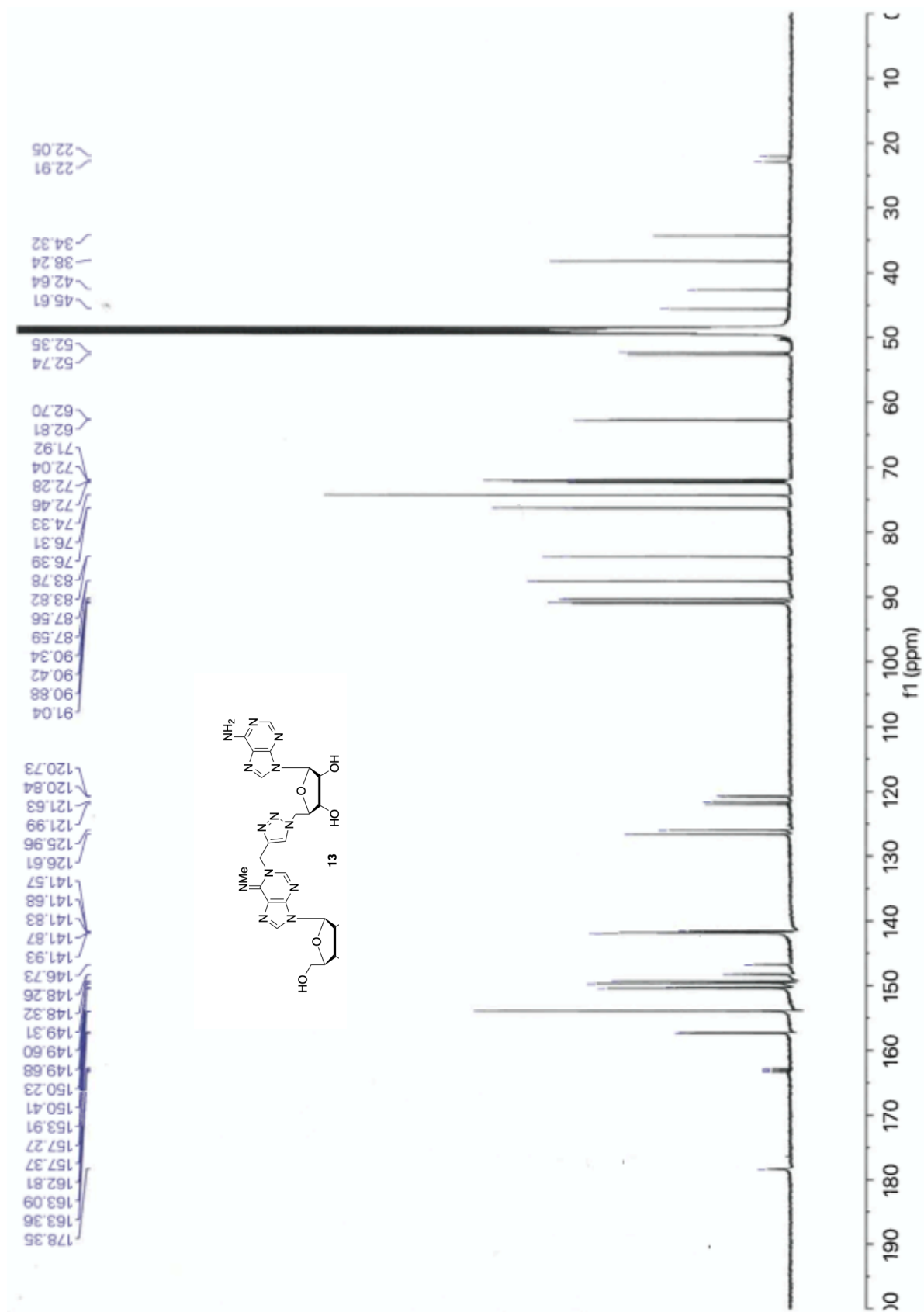
2. NMR spectra of final compounds



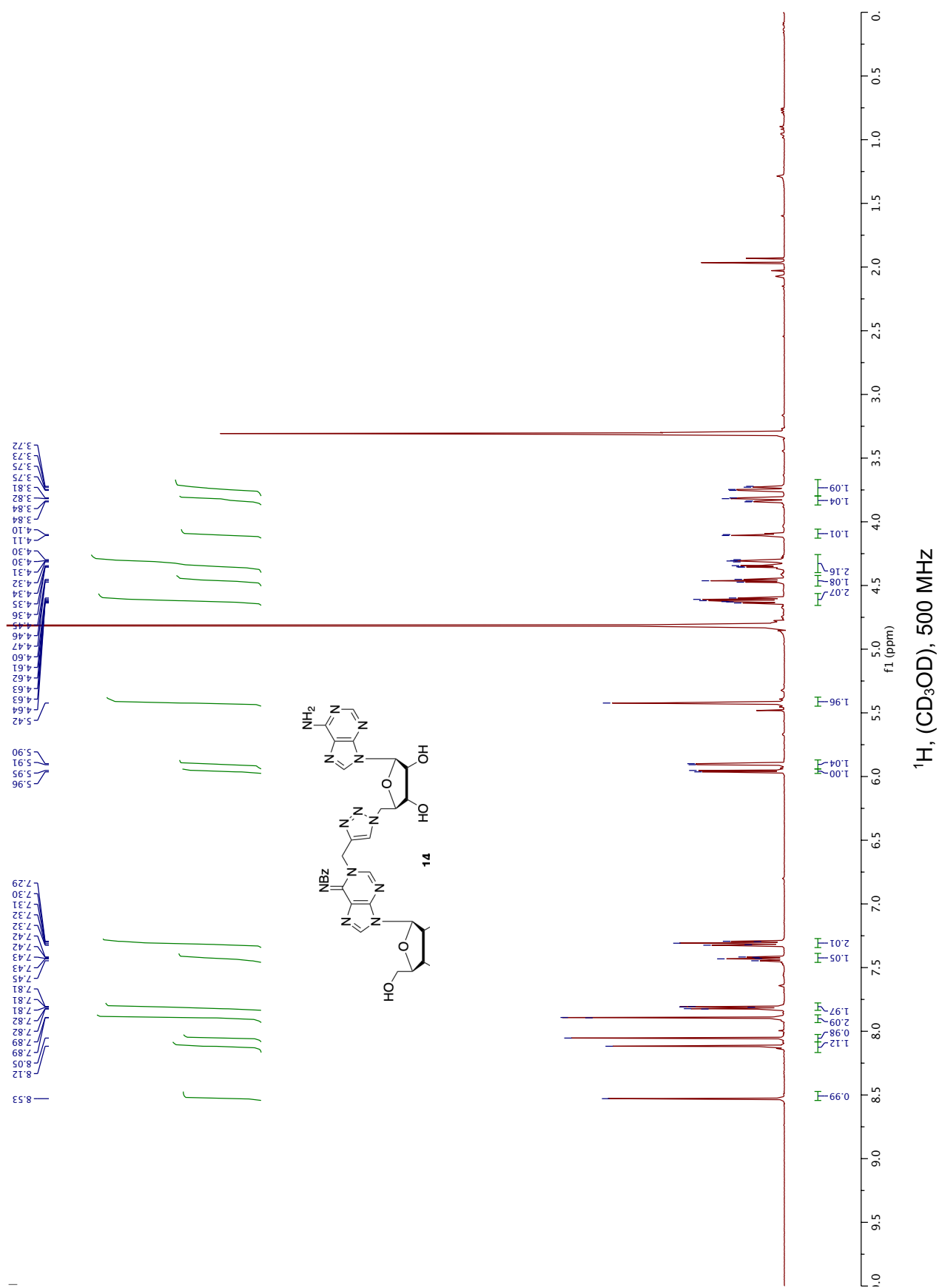


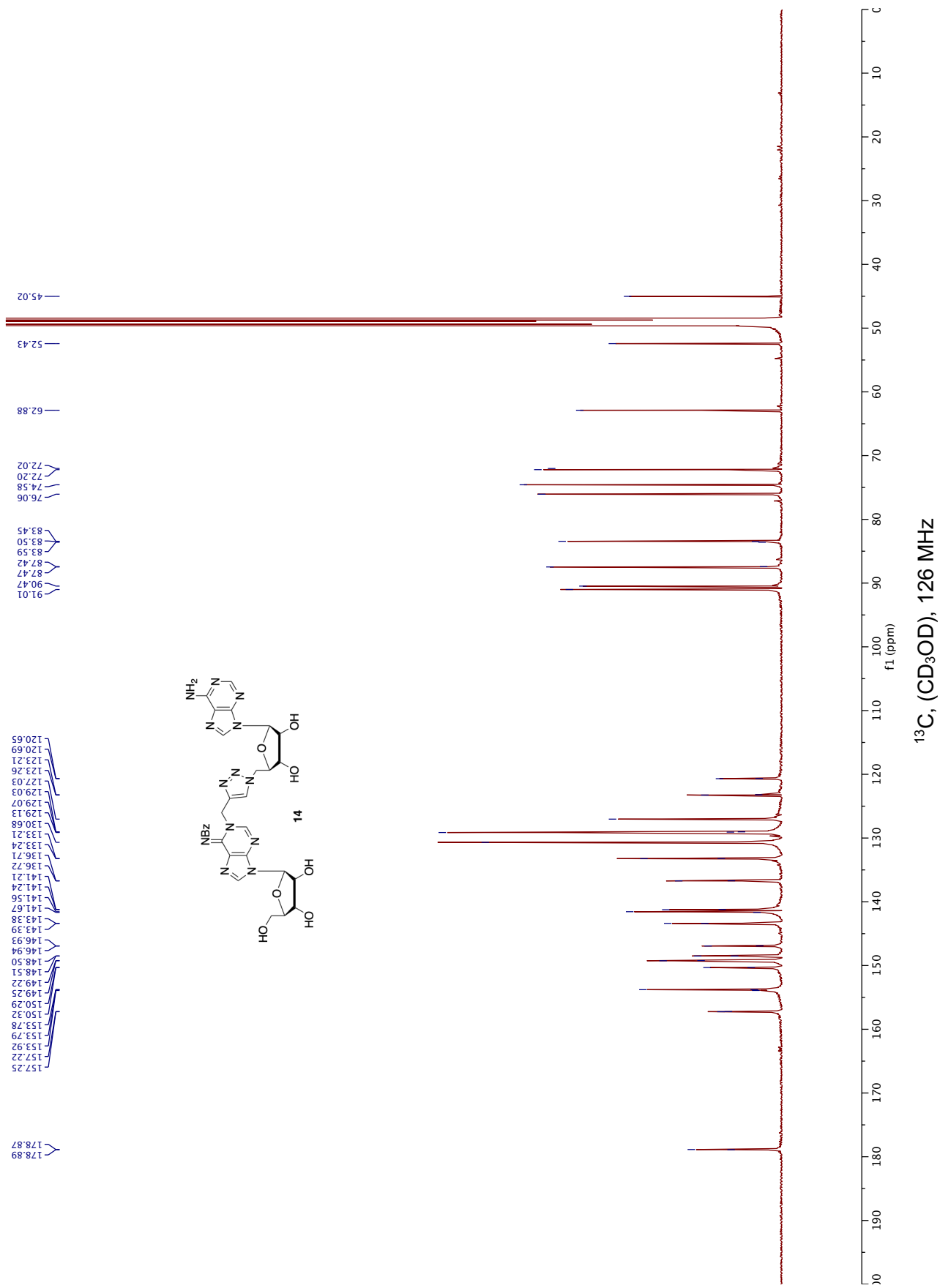


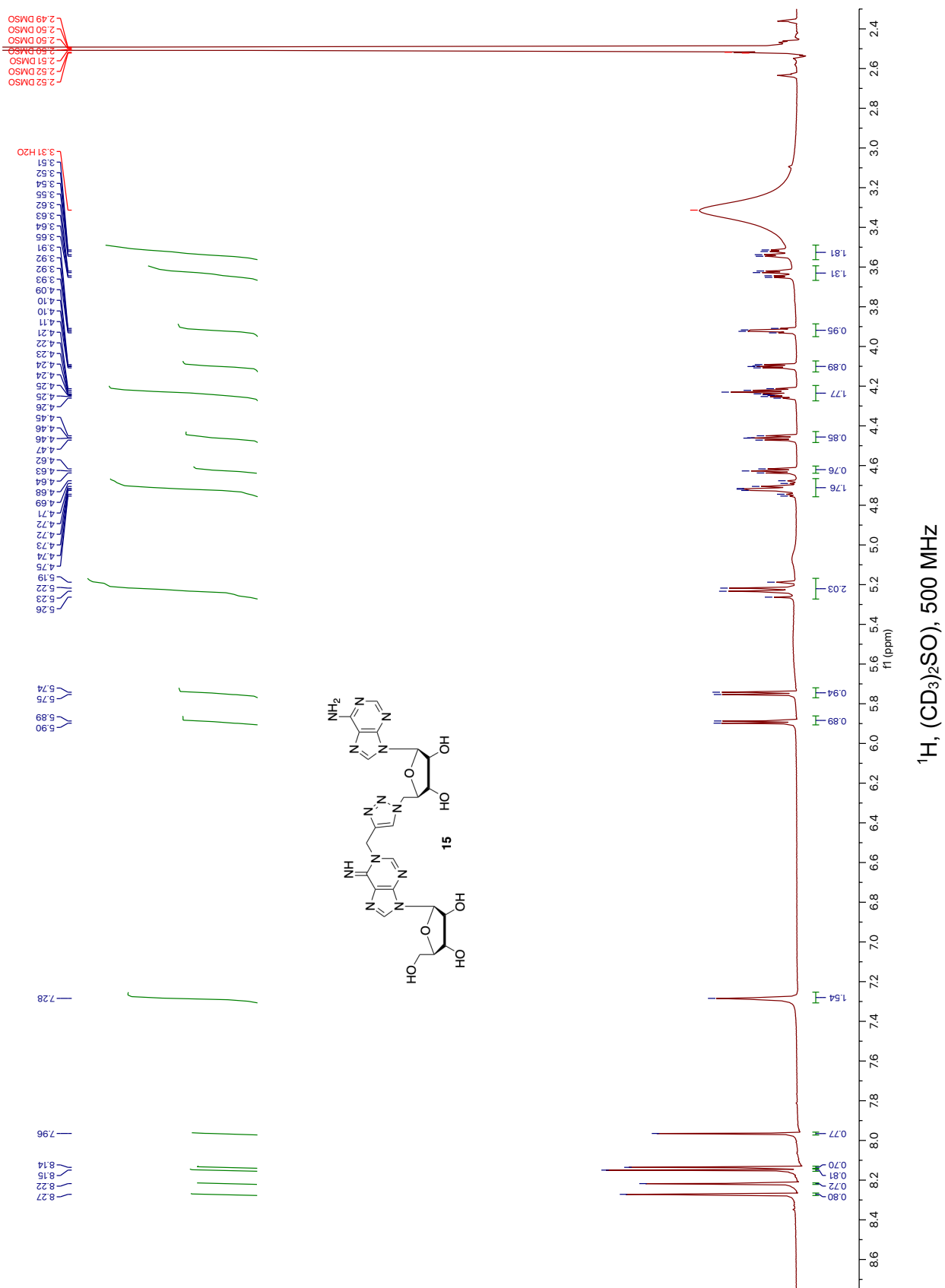
¹H, (CD₃OD), 500 MHz

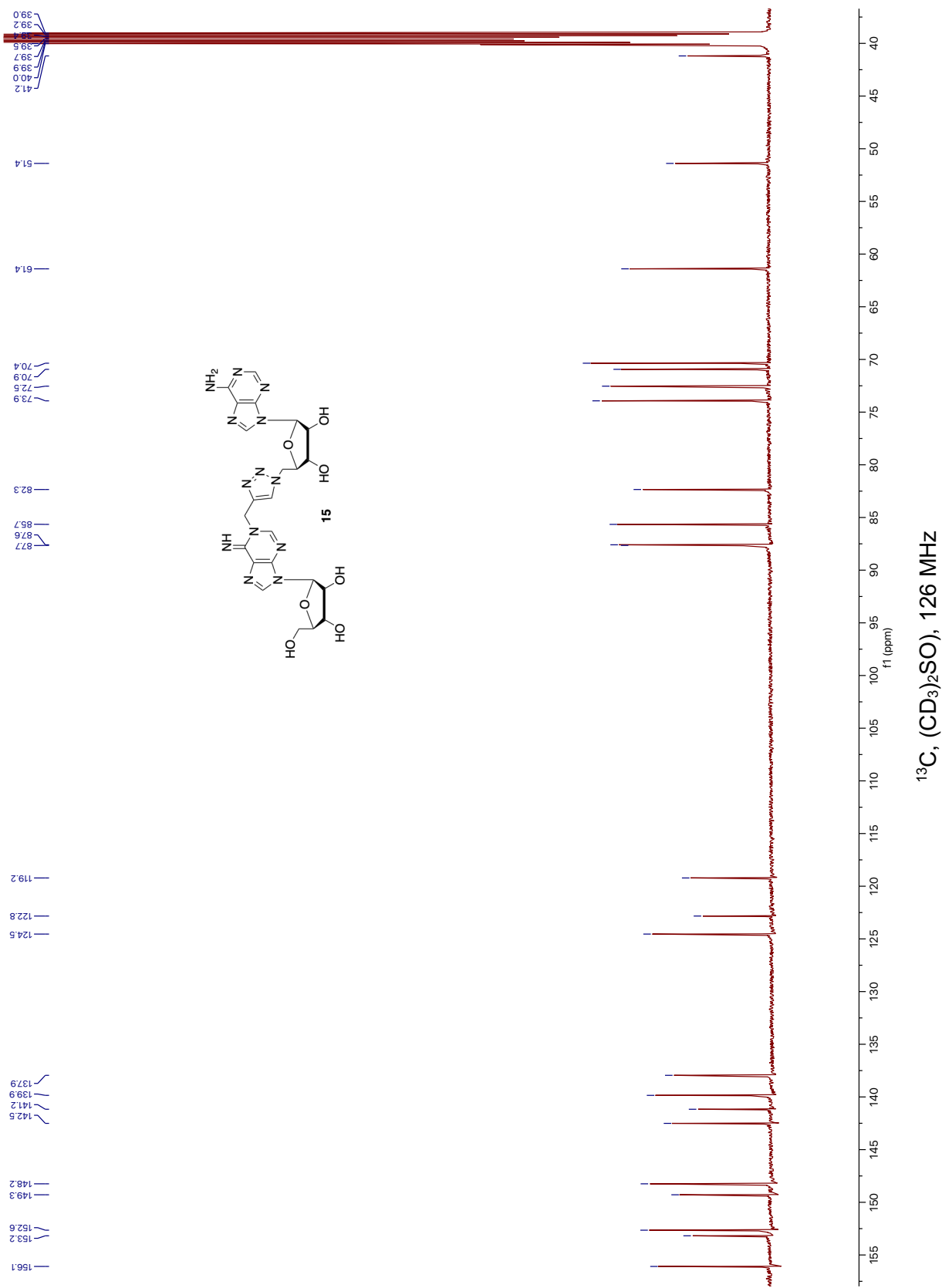


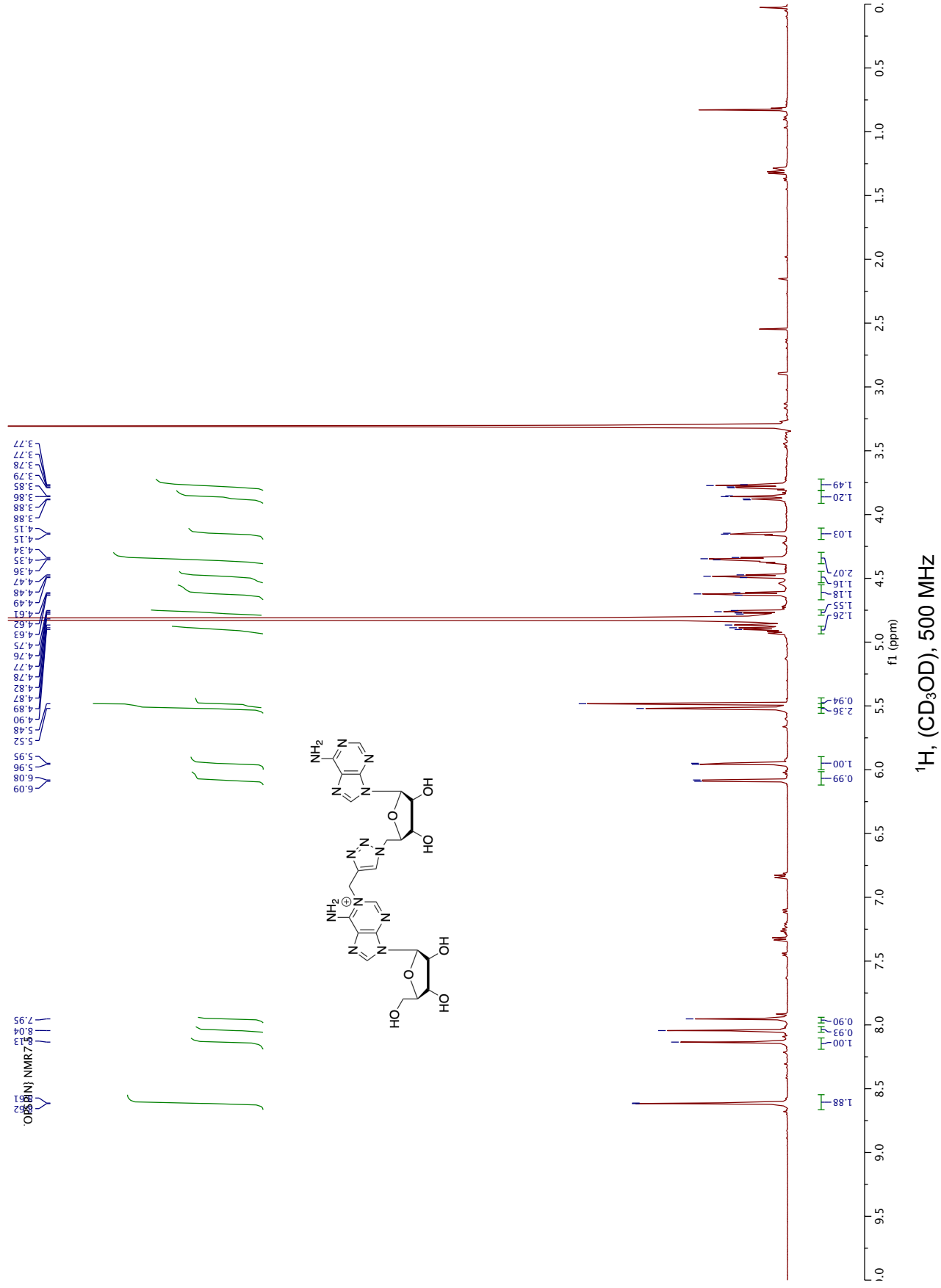
¹³C, (CD₃OD), 126 MHz



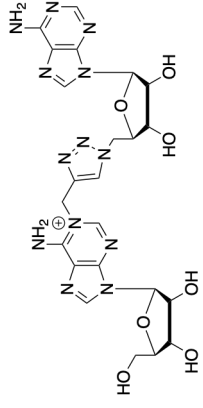




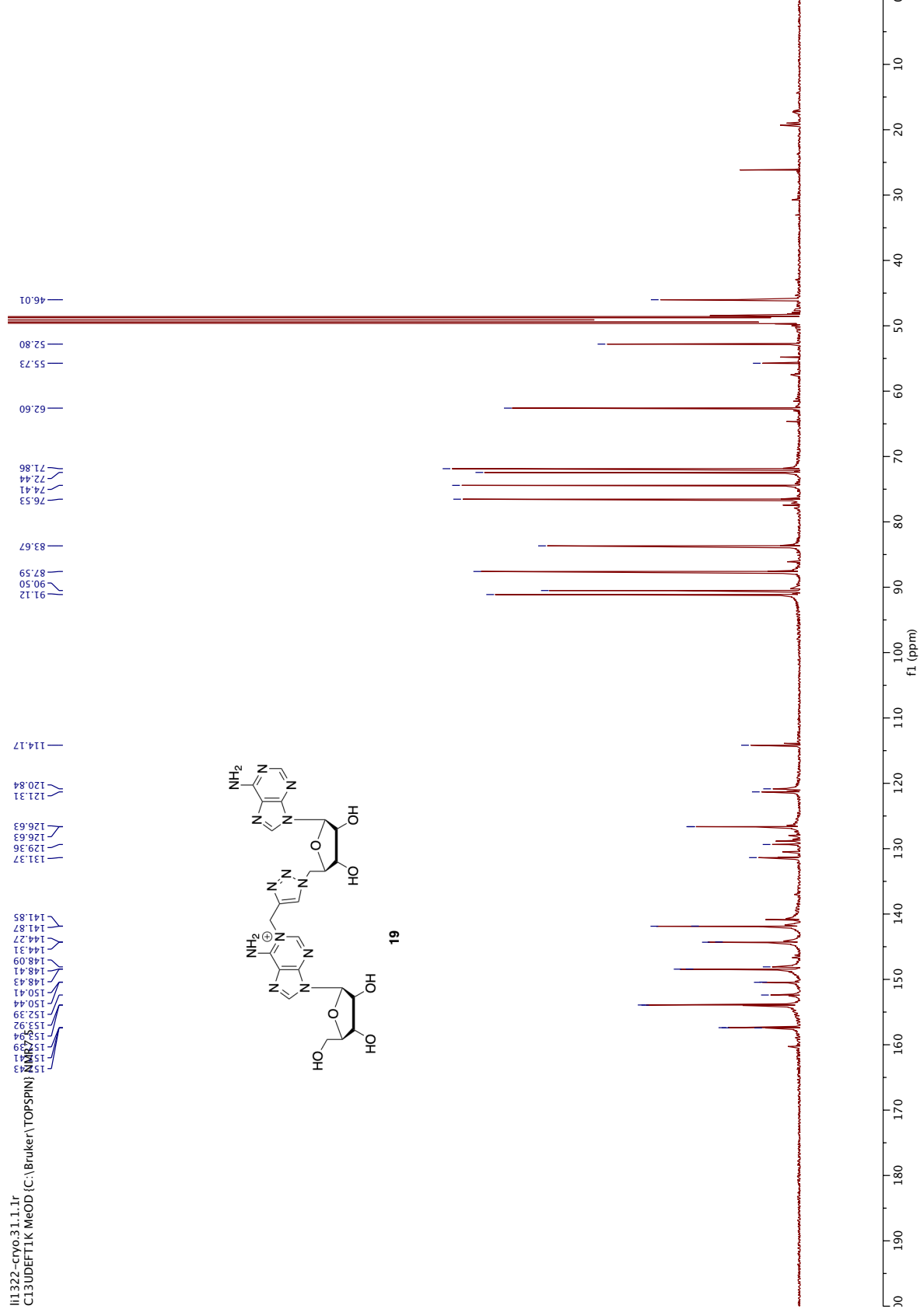




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li1322-cryo.31.1.1r
C13UDEFT1K MeOD {C:\Bruker\TOPSPIN}
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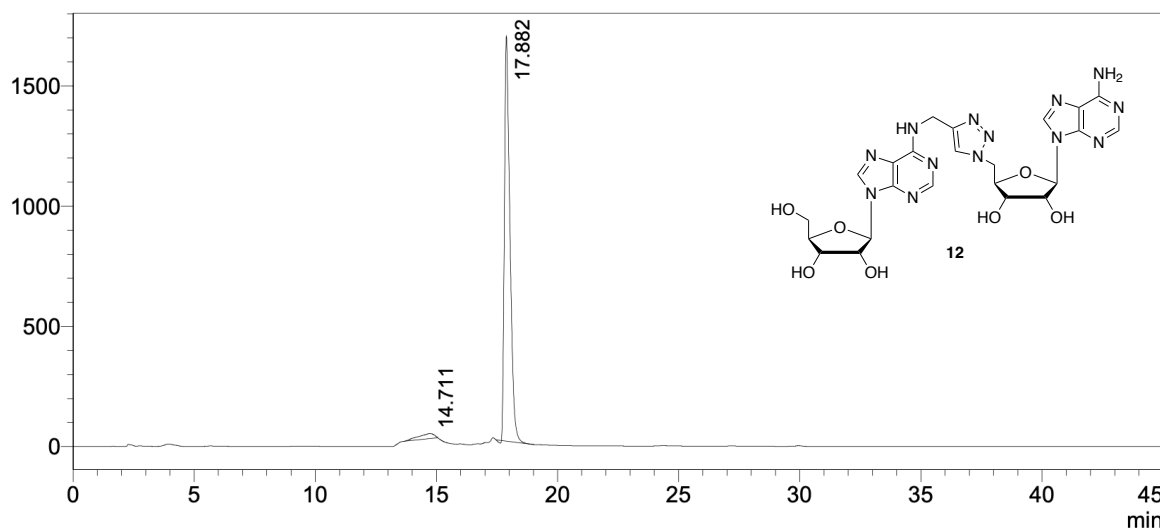


19

¹³C, (CD₃OD), 126 MHz

3. HPLC spectra of final compounds

mAU



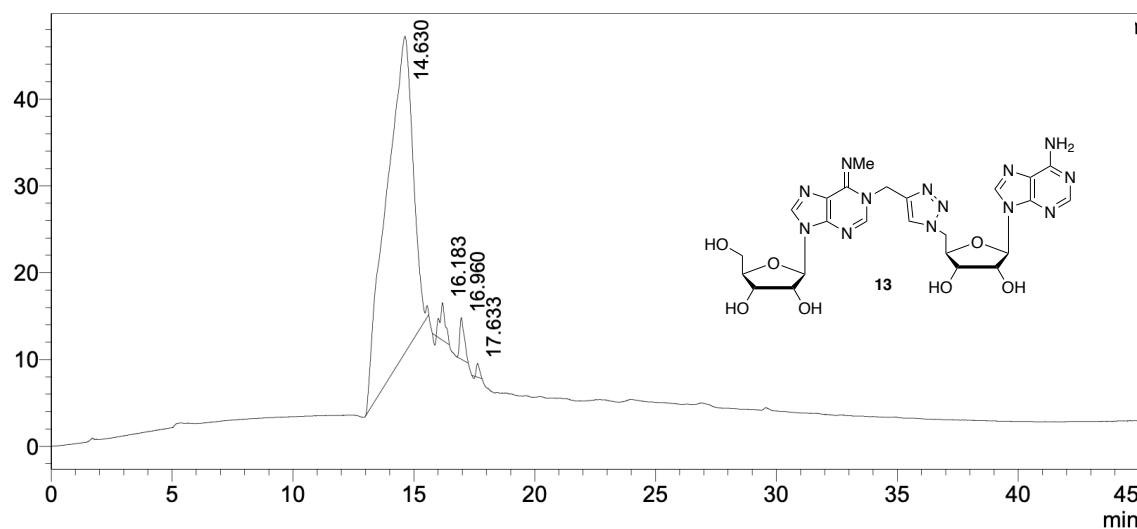
Peak#	Ret. Time	Area	Height	Conc.
1	14.711	1006582	20864	3.628
2	17.882	26738595	1684634	96.372
Total		27745177	1705497	

C18 100-5 NUCLEOSIL (Macherey Nagel), 25 mm X 4.6 mm, 5 μ m.

Flow: 1 mL/min; gradient: 0 to 100 % B in 30 min (A: H₂O; B: MeCN).

Detection 254 nm.

mAU



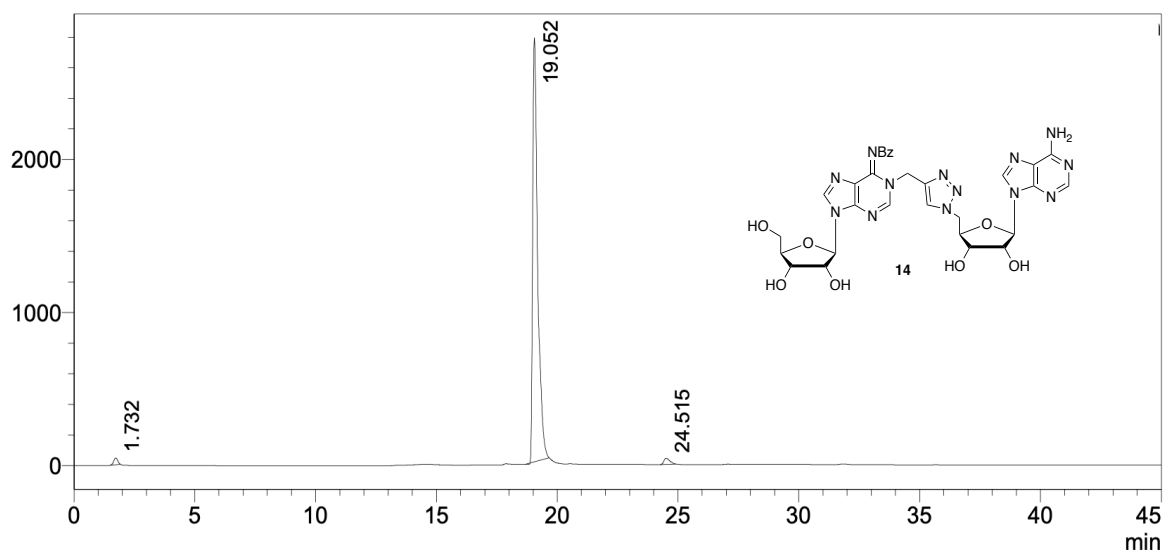
Peak#	Ret. Time	Area	Height	Conc.
1	14.630	2831932	36452	95.346
2	16.183	62509	4320	2.105
3	16.960	62520	4795	2.105
4	17.633	13191	1577	0.444
Total		2970152	47145	

C18 100-5 NUCLEOSIL (Macherey Nagel), 25 mm X 4.6 mm, 5 μ m.

Flow: 1 mL/min; gradient: 0 to 100 % B in 30 min (A: H₂O; B: MeCN).

Detection 254 nm.

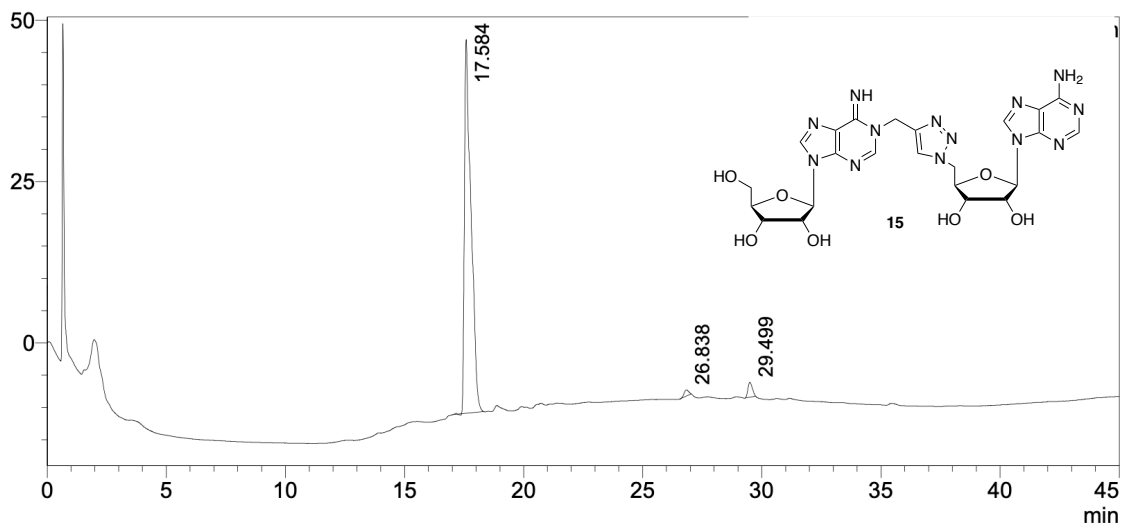
mAU



Peak#	Ret. Time	Area	Height	Conc.
1	1.732	506799	43757	1.249
2	19.052	39396210	2769417	97.112
3	24.515	664968	39548	1.639
Total		40567976	2852722	

C18 100-5 NUCLEOSIL (Macherey Nagel), 25 mm X 4.6 mm, 5 μ m.
 Flow: 1 mL/min; gradient: 0 to 100 % B in 30 min (A: H₂O; B: MeCN).
 Detection 214 nm.

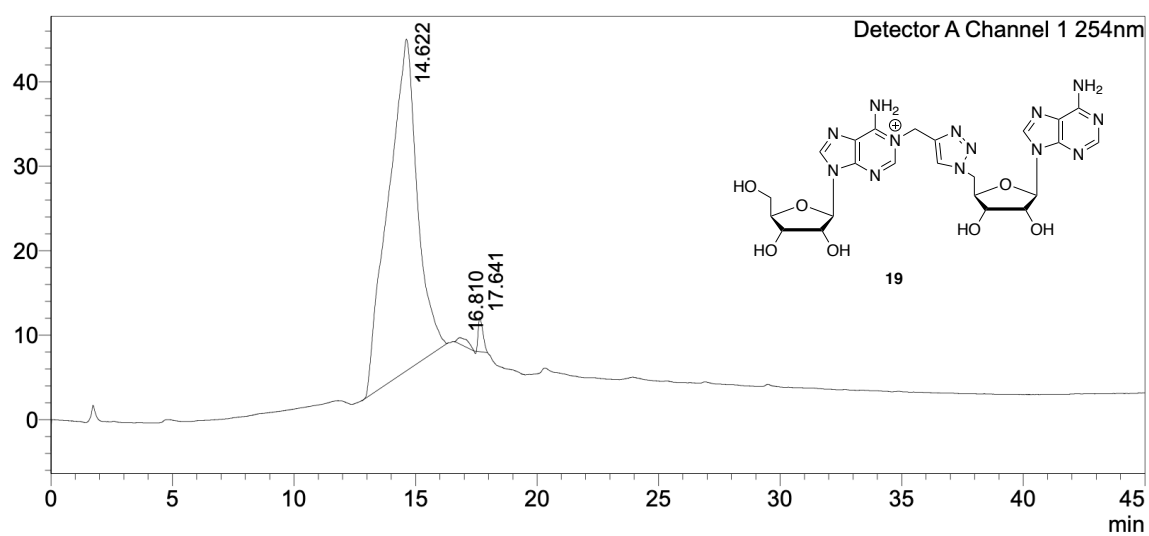
mAU



Peak#	Ret. Time	Area	Height	Conc.
1	17.584	1102188	57894	96.275
2	26.838	13201	972	1.153
3	29.499	29450	2288	2.572
Total		1144838	61155	

C18 100-5 NUCLEOSIL (Macherey Nagel), 25 mm X 4.6 mm, 5 μ m.
 Flow: 1 mL/min; gradient: 0 to 100 % B in 30 min (A: H₂O; B: MeCN).
 Detection 214 nm.

mAU



Peak#	Ret. Time	Area	Height	Conc.
1	14.622	3286323	39240	97.614
2	16.810	27588	745	0.819
3	17.641	52749	4035	1.567
Total		3366660	44021	

C18 100-5 NUCLEOSIL (Macherey Nagel), 25 mm X 4.6 mm, 5 μ m.
 Flow: 1 mL/min; gradient: 0 to 100 % B in 30 min (A: H₂O; B: MeCN).
 Detection 254 nm.