Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

Parallel-stranded DNA: Enhancing duplex stability by the 'G-clamp' and a pyrrolo-dC derivative

Xin Ming,[1] Ping Ding,[1,2] Peter Leonard,[1] Simone Budow[1] and Frank Seela[1,2]*

[1]Laboratory of Bioorganic Chemistry and Chemical Biology, Center for Nanotechnology, Heisenbergstrasse 11, 48149 Münster, Germany and [2]Laboratorium für Organische und Bioorganische Chemie, Institut für Chemie, Universität Osnabrück, Barbarastrasse 7, 49069 Osnabrück, Germany

Corresponding author:

Prof. Dr. Frank Seela

Phone: +49 (0)251-53406-500

Fax: +49 (0)251-53406-587

E-mail: Frank.Seela@uni-osnabrueck.de

Home page: www.seela.net

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Table S1. ^{1}H-^{13}C-coupling constants of compounds **6**, **13** and **15**.[a,b]

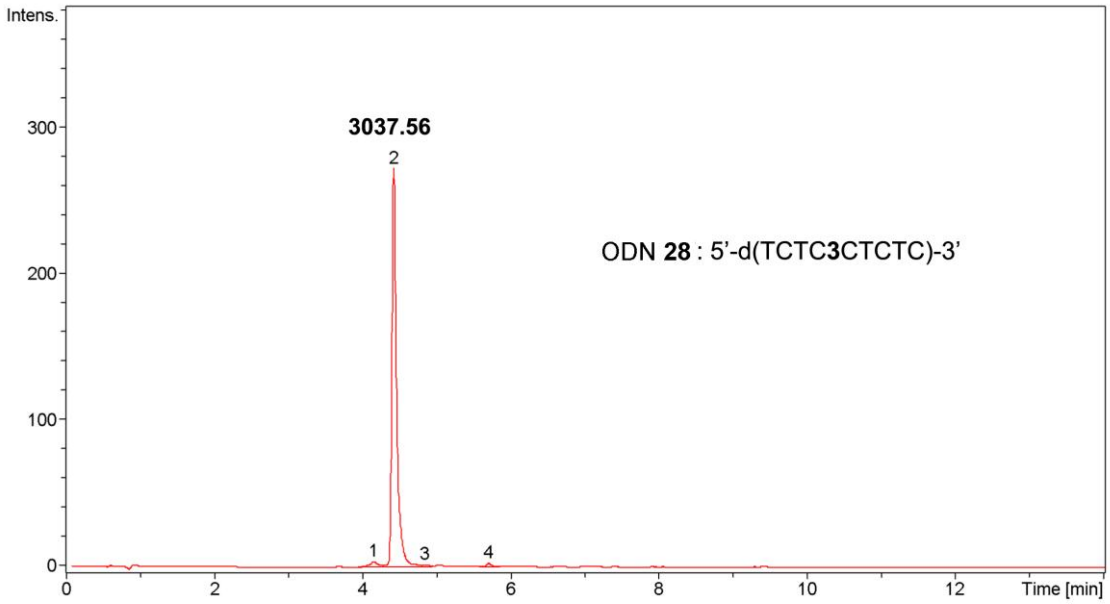
^{1}H-^{13}C coupling constants	*J* [Hz]		
	6	**13**	**15**
^{1}J(C4, H-C4)	187.4	-	182.6
^{2}J(C4a, H-C4)	3.6	-	-
^{3}J(C7a, H-C4)	7.1	-	7.5
^{1}J(C5, H-C5)	185.4	-	178.8
^{2}J(C4a, H-C5)	3.6	-	-
^{3}J(C7a, H-C5)	7.1	-	7.5
^{2}J(C6, H-C5)	5.0	-	9.8
^{1}J(C1', H-C1')	173.5	-	174.6
^{1}J(C3', H-C3')	147.3	-	148.1
^{1}J(C4', H-C4')	146.3	-	146.3
^{1}J(C5', H-C5')	139.4	-	141.3
^{1}J(C1'', H-C1'')	-	142.1	142.1
^{1}J(C2'', H-C2'')	-	129.8	130.1
^{1}J(C3'', H-C3'')	-	139.1	139.3

[a] Measured in DMSO-d_6 at 298 K. [b] Systematic numbering.

Table S2. Molecular masses of oligonucleotides determined by mass spectrometry.

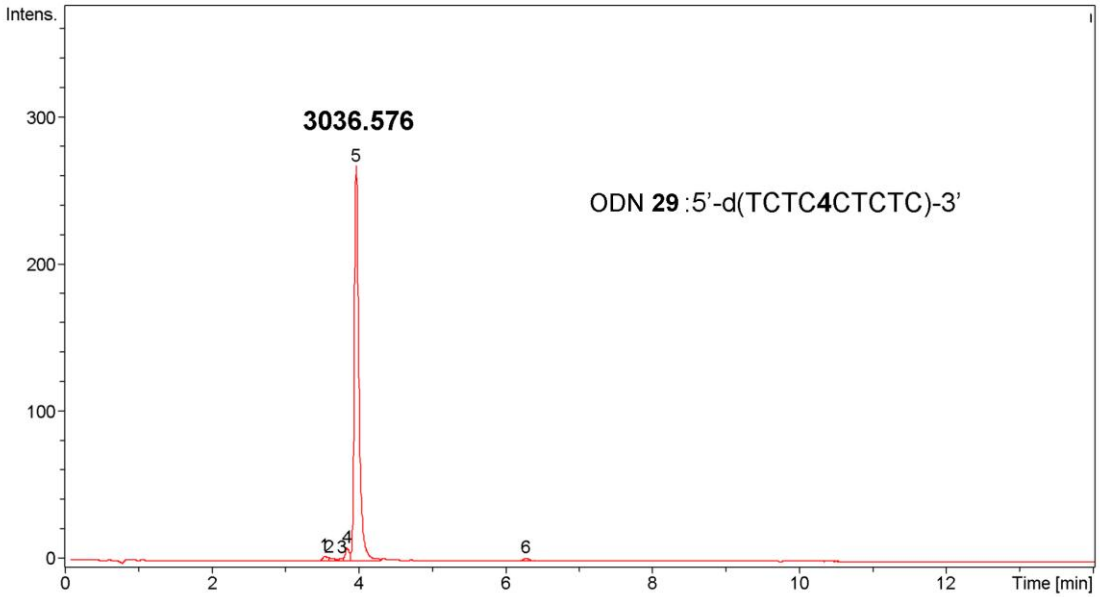
	Sequence	Mol. Wt. (calc.)	Mol. Wt. (found)
ODN-**28**	5'-d(TCTC**3**CTCTC)-3'	3038	3038[a]
ODN-**29**	5'-d(TCTC**4**CTCTC)-3'	3037	3037[a]
ODN-**33**	5'-d(TT**1** TTT TTT TAT TAA AAT TTA T**1**A A)-3'	7665	7664[b]
ODN-**34**	5'-d(AA**3** AAA AAA ATA ATT TTA AAT A**3**T T)-3'	7945	7948[c]
ODN-**35**	5'-d(AA**4** AAA AAA ATA ATT TTA AAT A**4**T T)-3'	7944	7944[c]

[a] Measured by LC-ESI-TOF mass spectrometry. [b] Measured by MALDI-TOF mass spectrometry in the linear negative mode. [c] Measured by MALDI-TOF mass spectrometry in the linear positive mode.



#	RT [min]	Area Frac. %	Max. MW
1	4.2	2.3	3070.532
2	4.4	96.0	3037.561
3	4.8	0.7	3037.525
4	5.7	1.0	4729.804

Figure S1. LC-ESI-MS chromatogram of ODN-**28**.



#	RT [min]	Area Frac. %	Max. MW
1	3.5	1.2	2732.490
2	3.6	0.9	2747.488
3	3.8	0.6	
4	3.8	2.8	3036.556
5	4.0	93.7	3036.576
6	6.3	0.8	

Figure S2. LC-ESI-MS chromatogram of ODN-**29**.

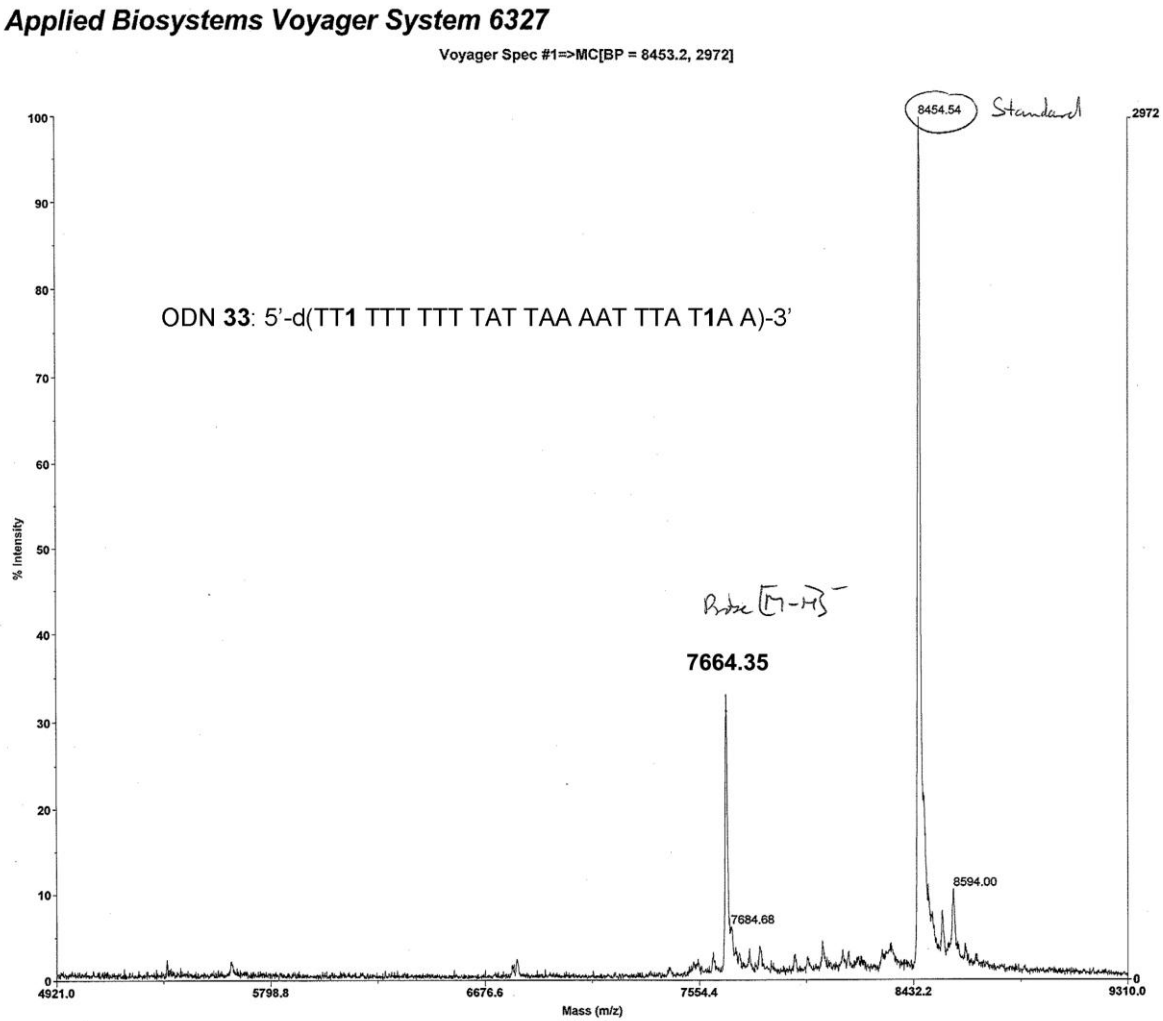


Figure S3. Maldi-TOF mass spectrum of ODN-**33**.

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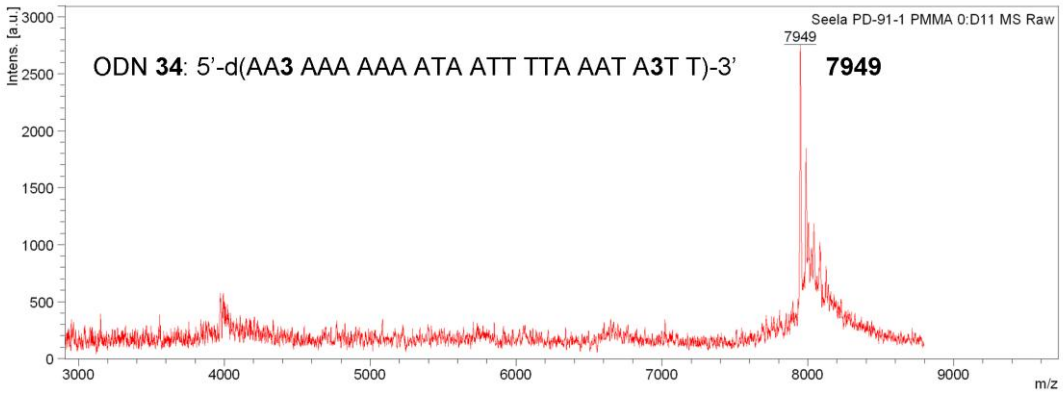


Figure S4. Maldi-TOF mass spectrum of ODN-**34**.

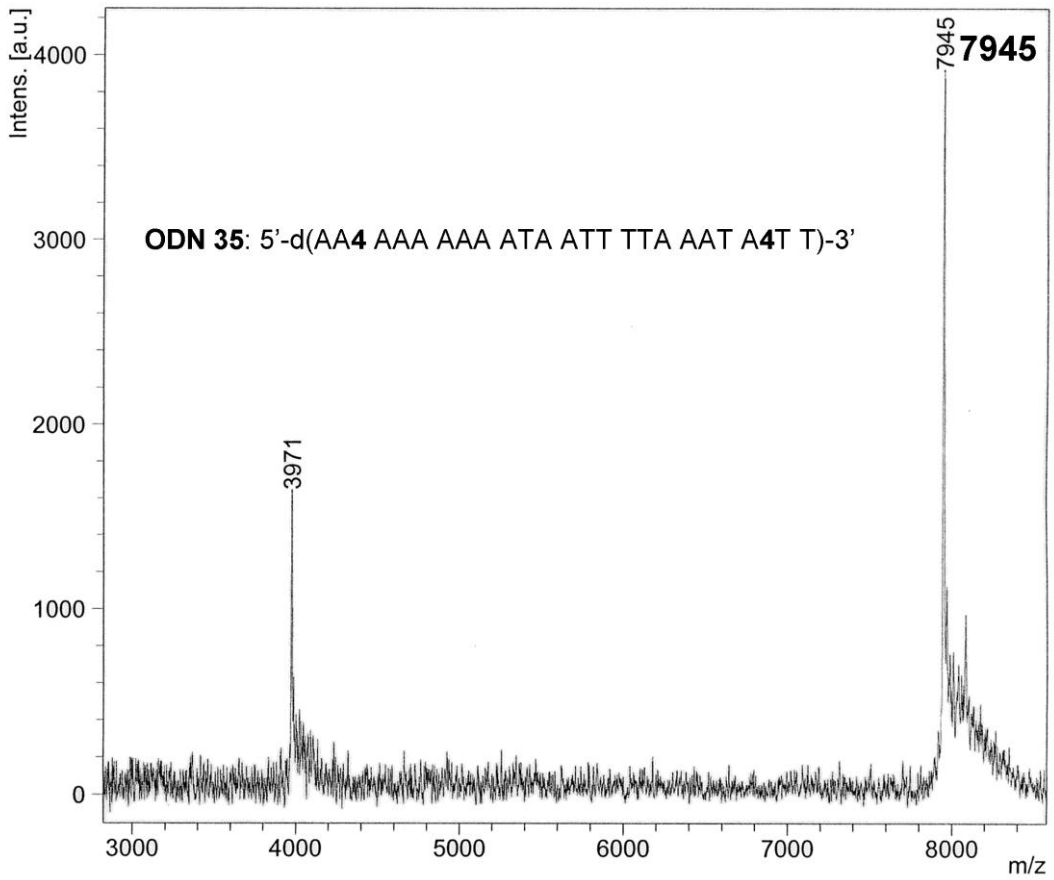


Figure S5. Maldi-TOF mass spectrum of ODN-**35**.

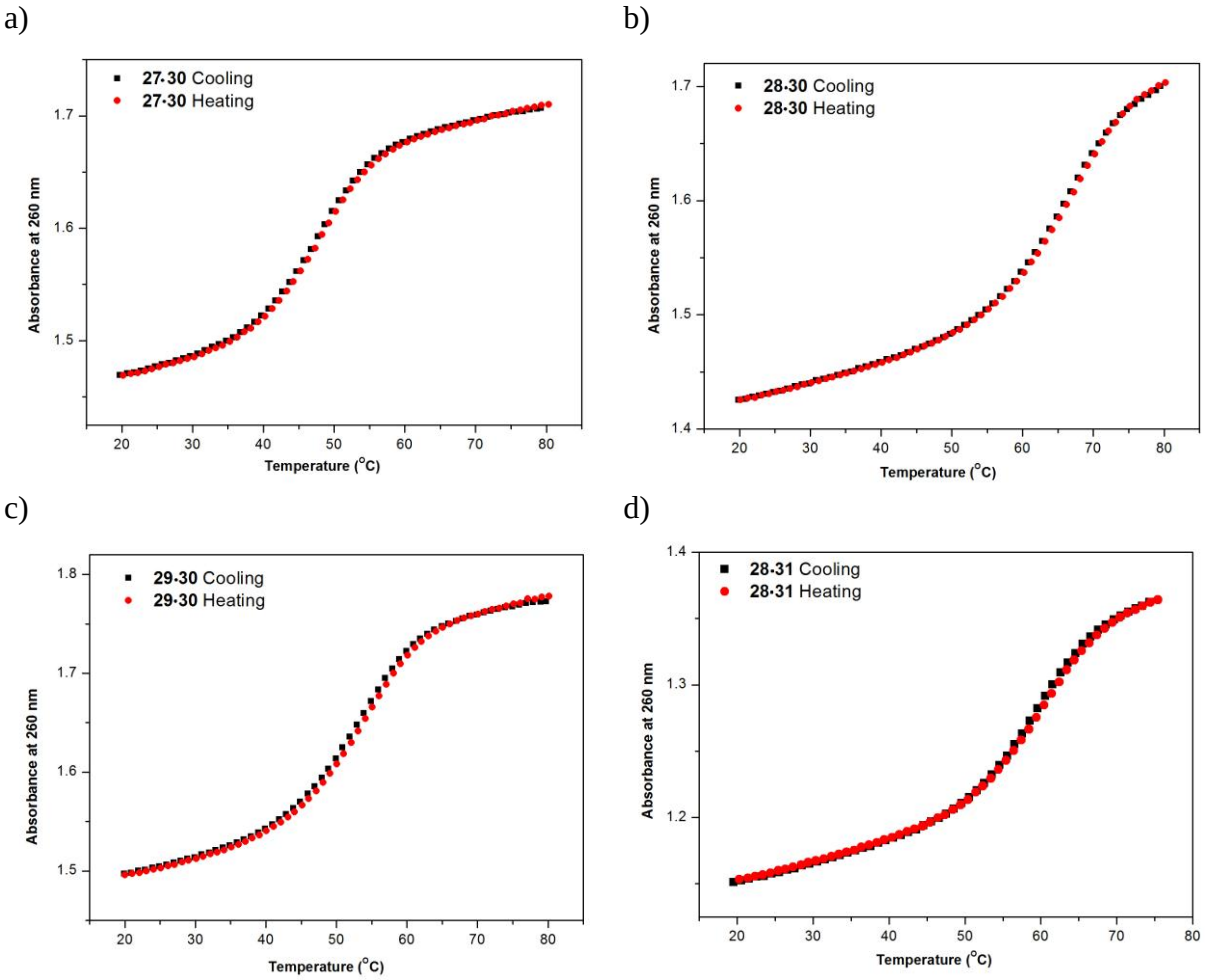
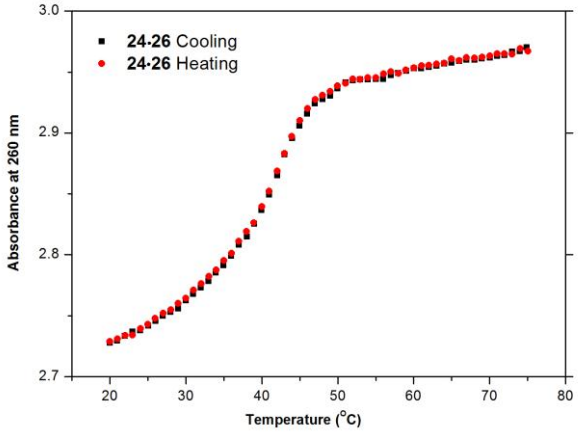


Figure S6. Melting curves of parallel stranded duplexes obtained from cooling (black square) and heating (red circle) experiments monitored at 260 nm and measured in 0.1 M NaCl, 10 mM $MgCl_2$, 10 mM Na-cacodylate (pH 7.0) with 5 µM + 5 µM single-strand concentration. (a) Duplex **27•30**; (b) duplex **28•30**; (c) duplex **29•30** and (d) duplex **28•31**.

a)



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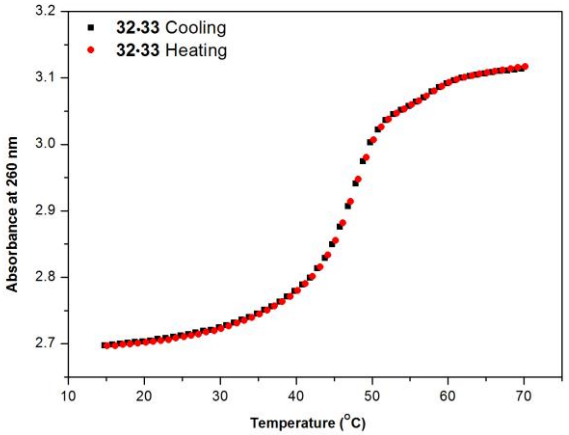
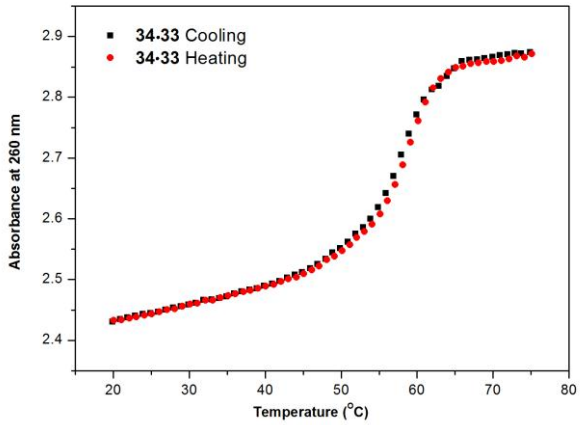


c)



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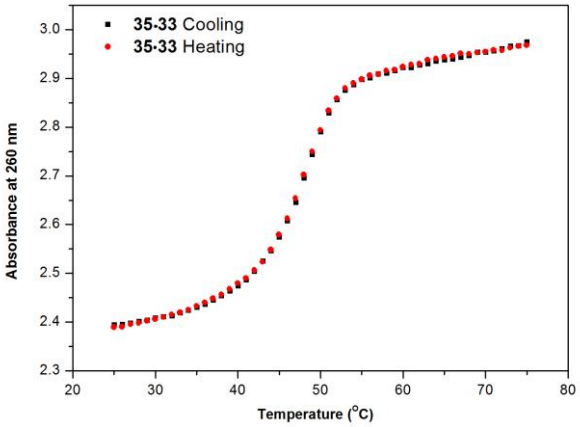
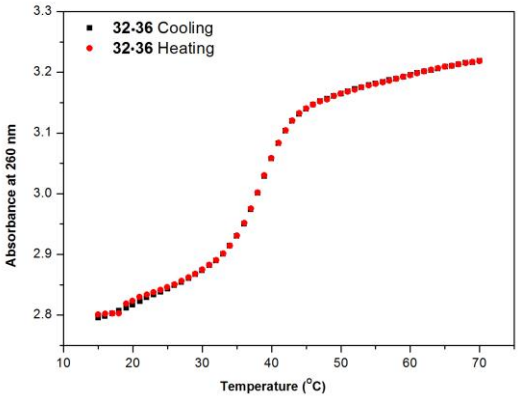


e)



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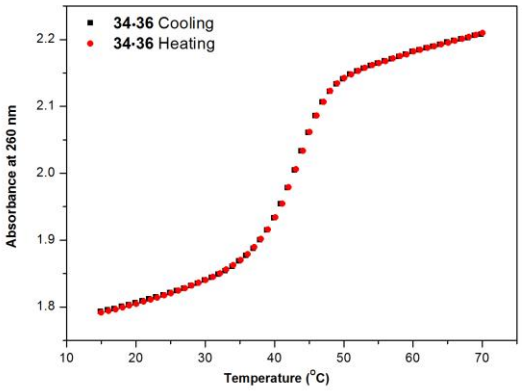

g)

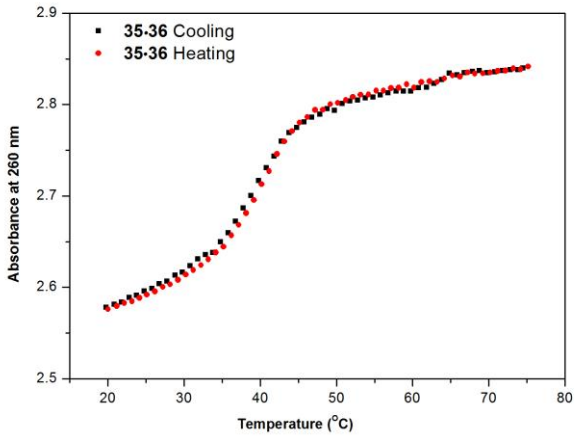

Figure S7. Melting curves of parallel stranded duplexes obtained from cooling (black square) and heating (red circle) experiments monitored at 260 nm and measured in 0.1 M NaCl, 10 mM $MgCl_2$, 10 mM Na-cacodylate (pH 7.0) with 5 µM + 5 µM single-strand concentration. (a) Duplex **24•26**; (b) duplex **32•33**; (c) duplex **34•33**; (d) duplex **35•33**; (e) duplex **32•36**; (f) duplex **34•36** and (g) duplex **35•36**.

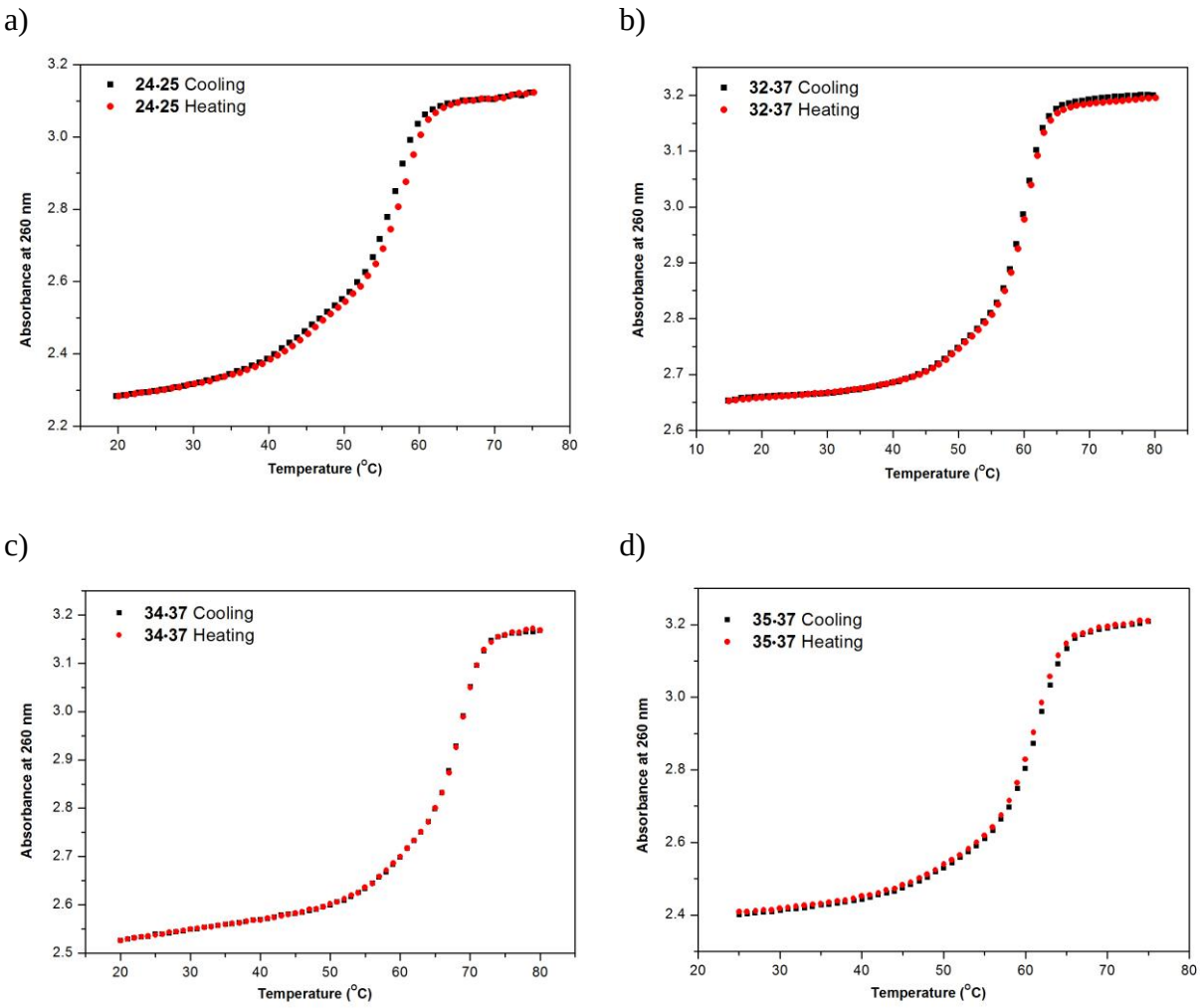

Figure S8. Melting curves of antiparallel stranded duplexes obtained from cooling (black square) and heating (red circle) experiments monitored at 260 nm and measured in 0.1 M NaCl, 10 mM $MgCl_2$, 10 mM Na-cacodylate (pH 7.0) with 5 μM + 5 μM single-strand concentration. (a) Duplex **24•25**; (b) duplex **32•37**; (c) duplex **34•37** and (d) duplex **35•37**.

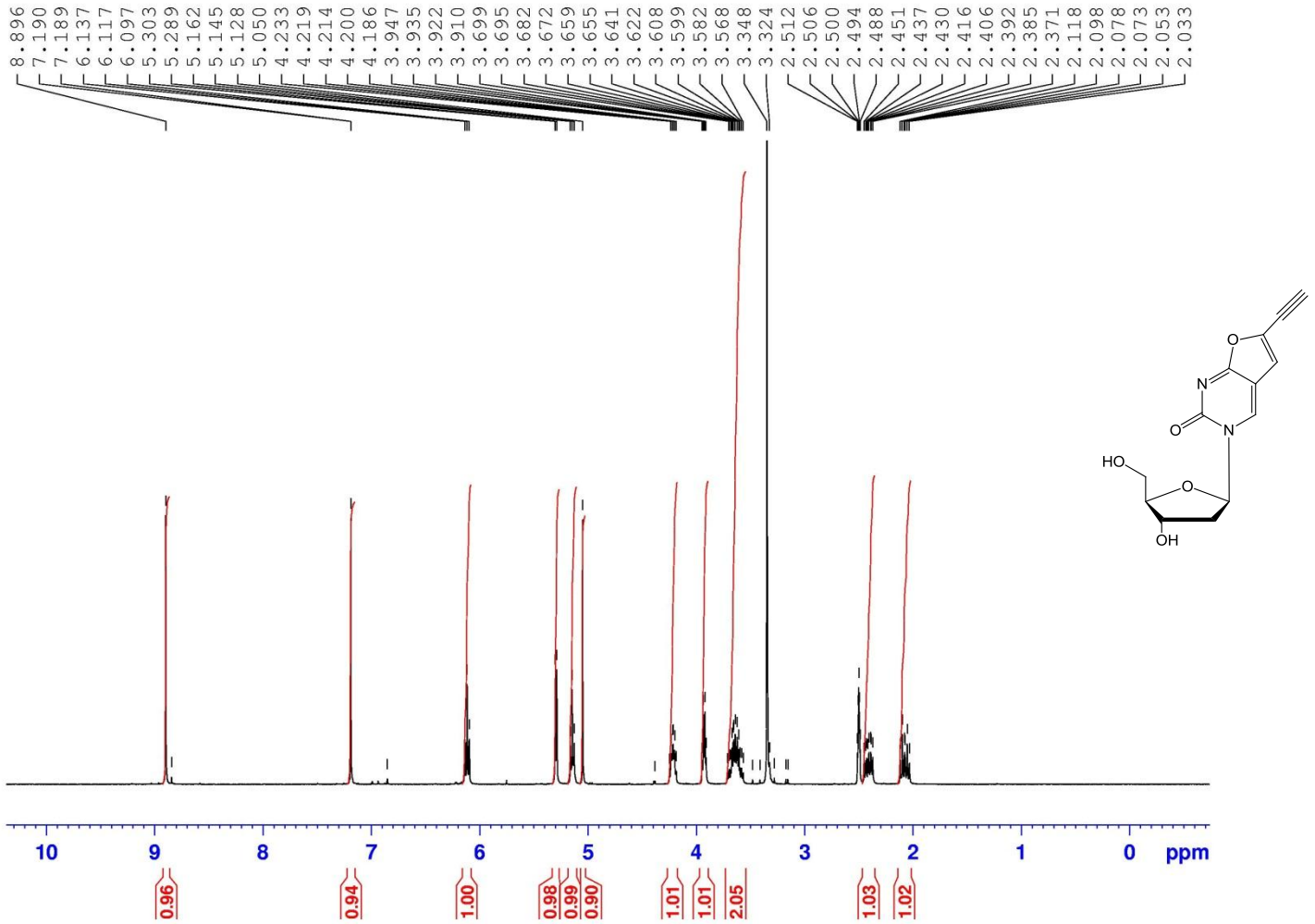

Figure S9. ^{1}H-NMR spectrum of 3-(2-deoxy-ß-D-*erythro*-pentofuranosyl)-6-ethynyl-furo[2,3-*d*]pyrimidin-2(3*H*)-one (**6**).

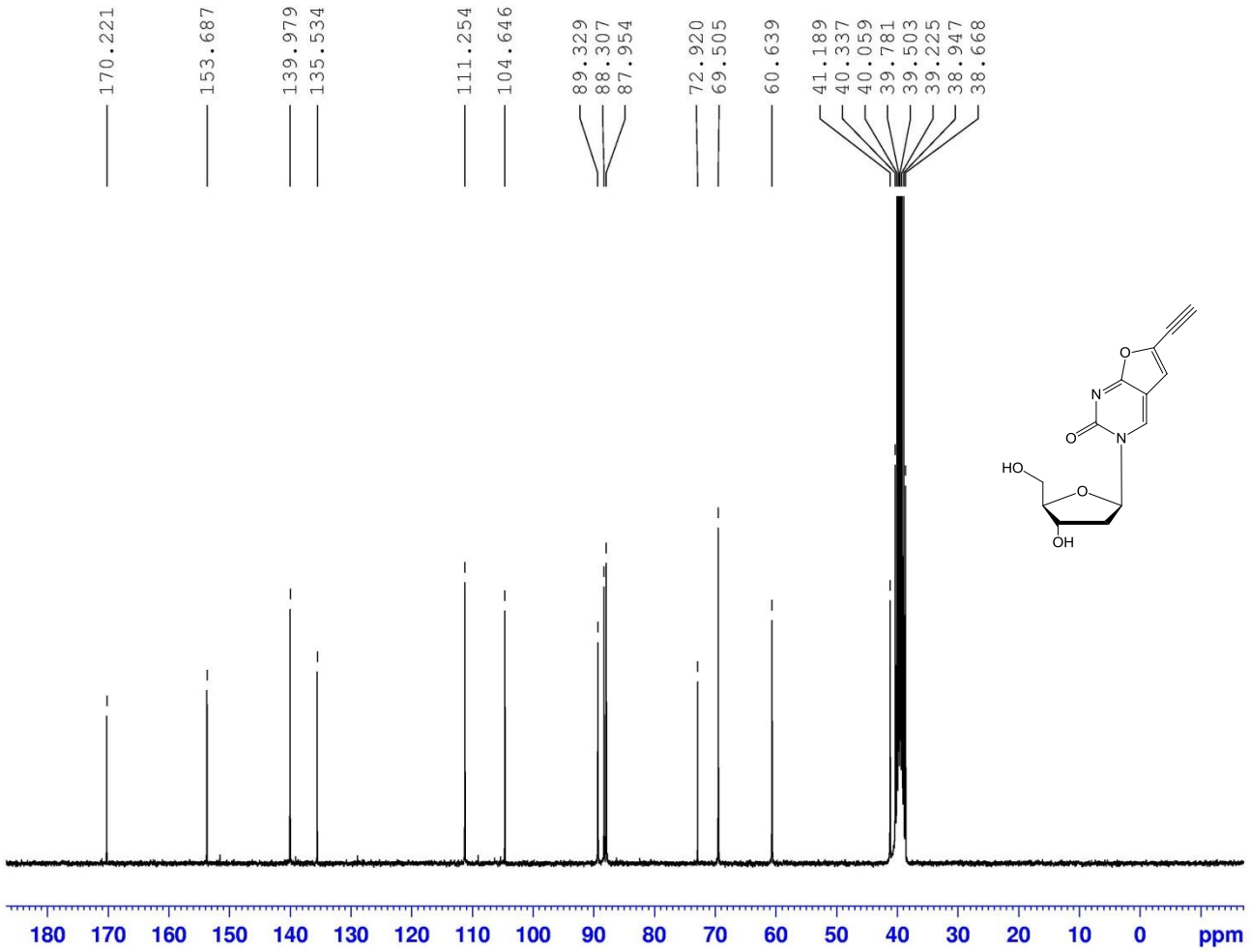

Figure S10. ^{13}C-NMR spectrum of 3-(2-deoxy-ß-D-*erythro*-pentofuranosyl)-6-ethynyl-furo[2,3-*d*]pyrimidin-2(3*H*)-one (**6**).

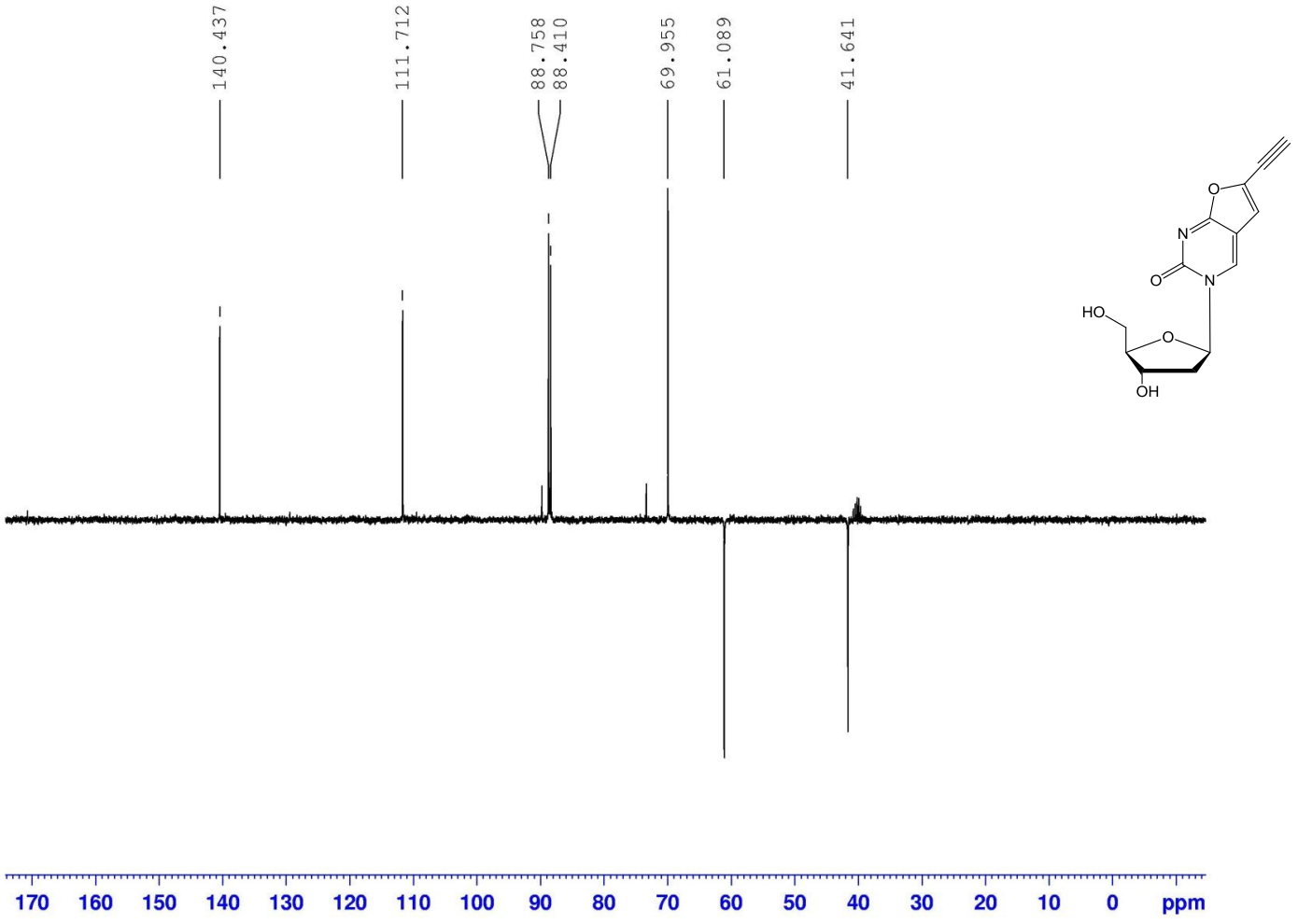

Figure S11. DEPT-135 spectrum of 3-(2-deoxy-ß-D-*erythro*-pentofuranosyl)-6-ethynyl-furo[2,3-*d*]pyrimidin-2(3*H*)-one (**6**).

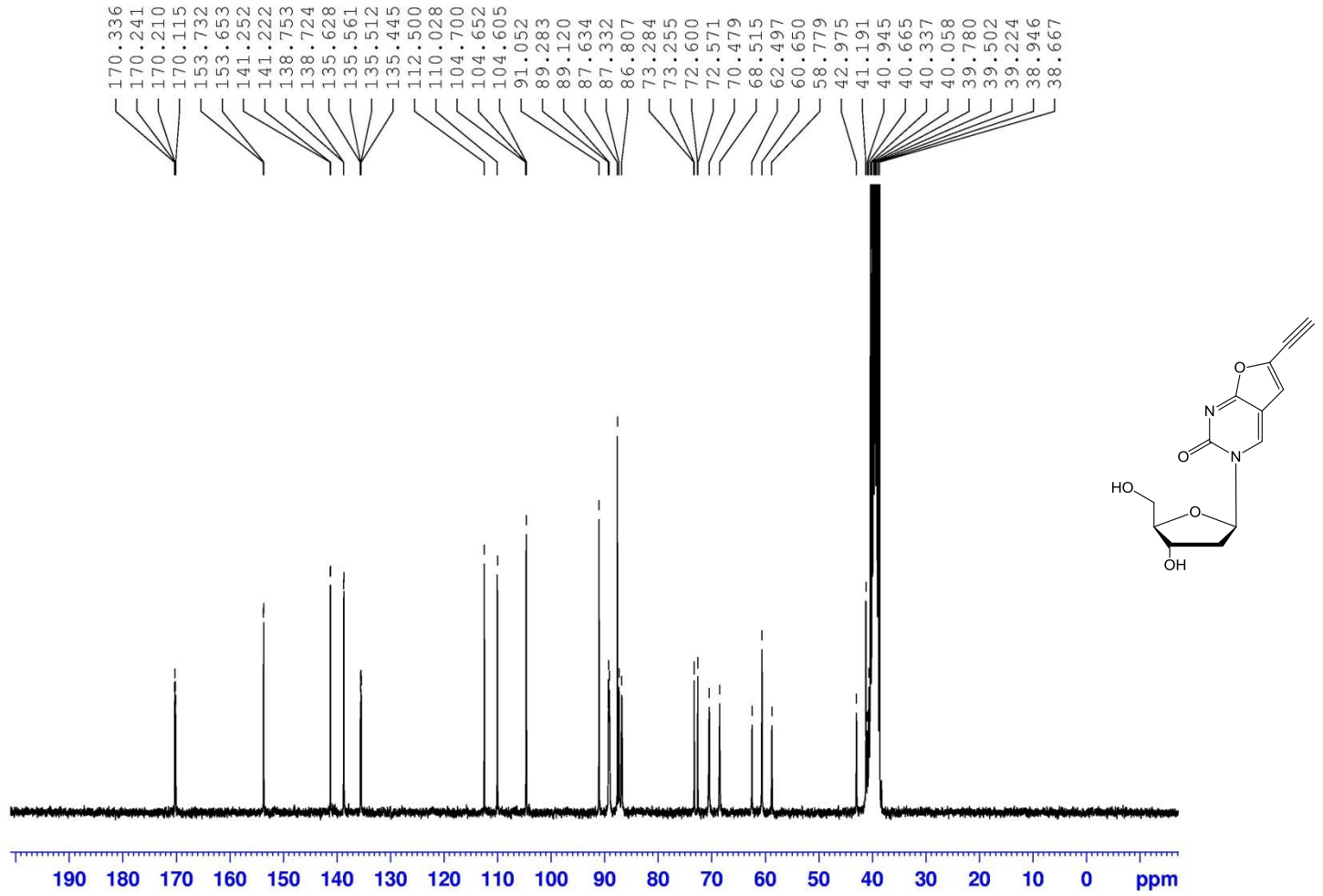

Figure S12. ^{1}H-^{13}C-gated decoupled spectrum of 3-(2-deoxy-*ß*-D-*erythro*-pentofuranosyl)-6-ethynyl-furo[2,3-*d*]pyrimidin-2(3*H*)-one (**6**).

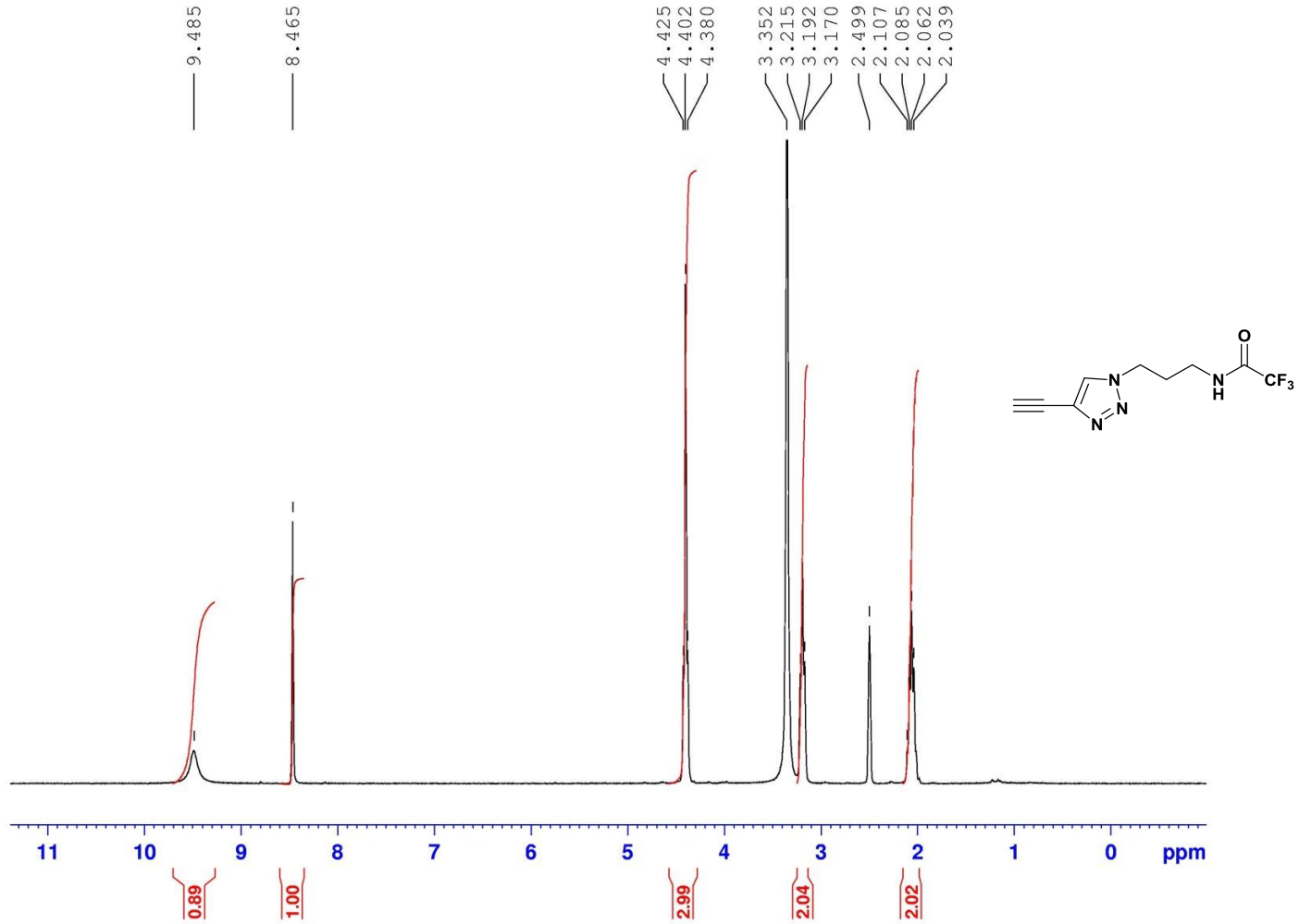

Figure S13. ^{1}H-NMR spectrum of *N*-(3-(4-ethynyl-1*H*-1,2,3-triazol-1-yl)propyl)-2,2,2-trifluoroacetamide (**13**).

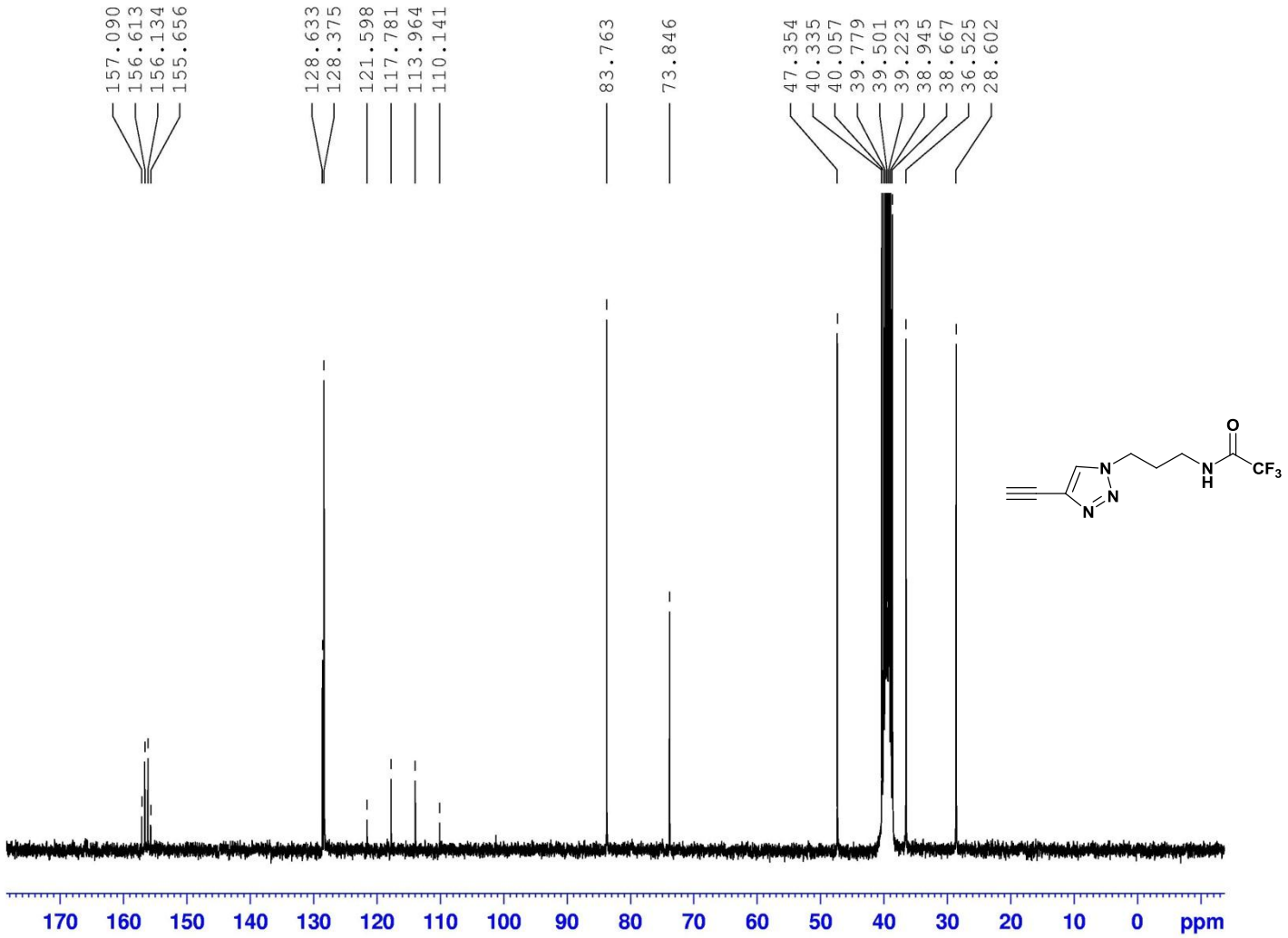

Figure S14. ^{13}C-NMR spectrum of *N*-(3-(4-ethynyl-1*H*-1,2,3-triazol-1-yl)propyl)-2,2,2-trifluoroacetamide (**13**).

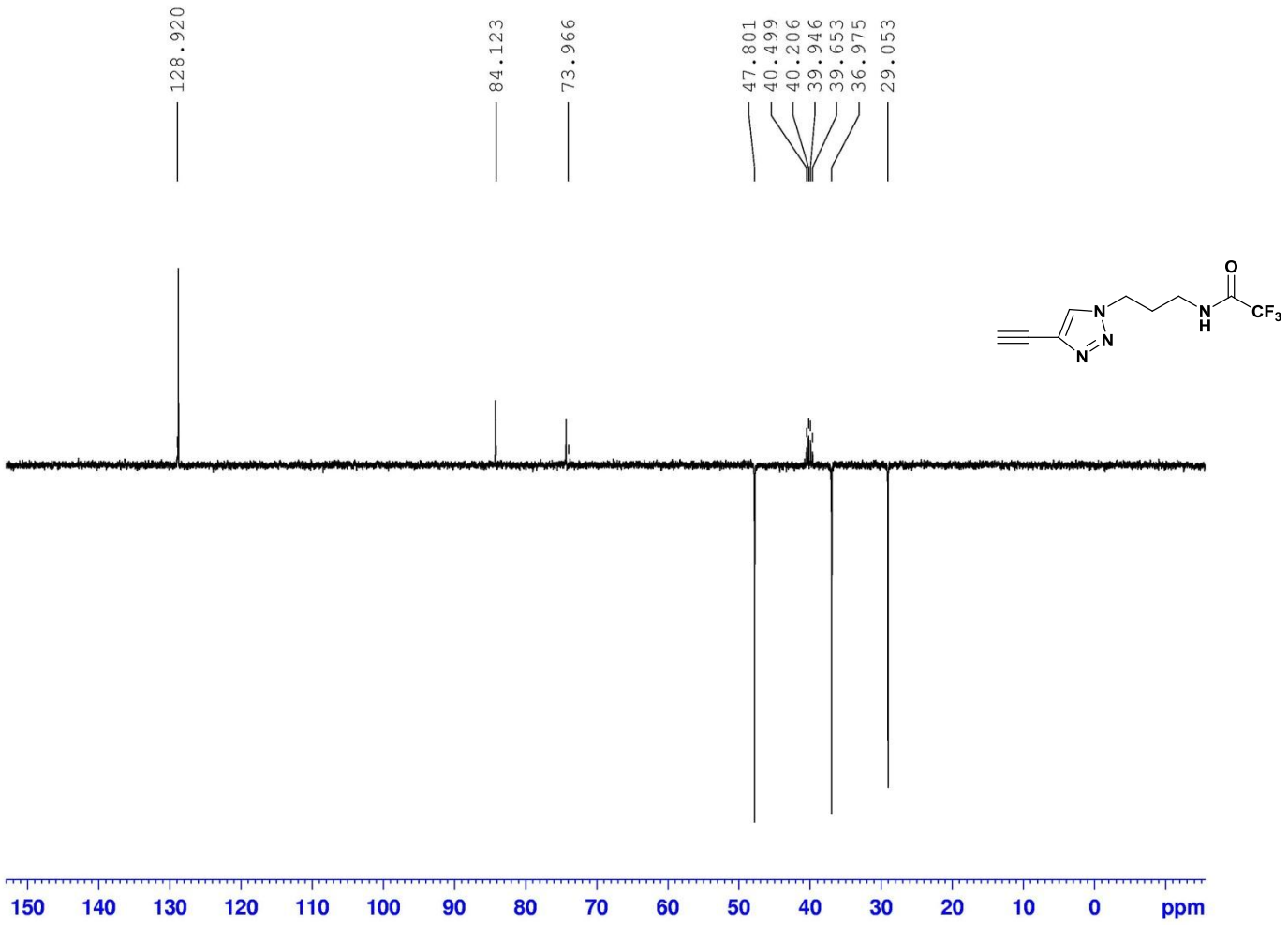

Figure S15. DEPT-135 spectrum of *N*-(3-(4-ethynyl-1*H*-1,2,3-triazol-1-yl)propyl)-2,2,2-trifluoroacetamide (**13**).

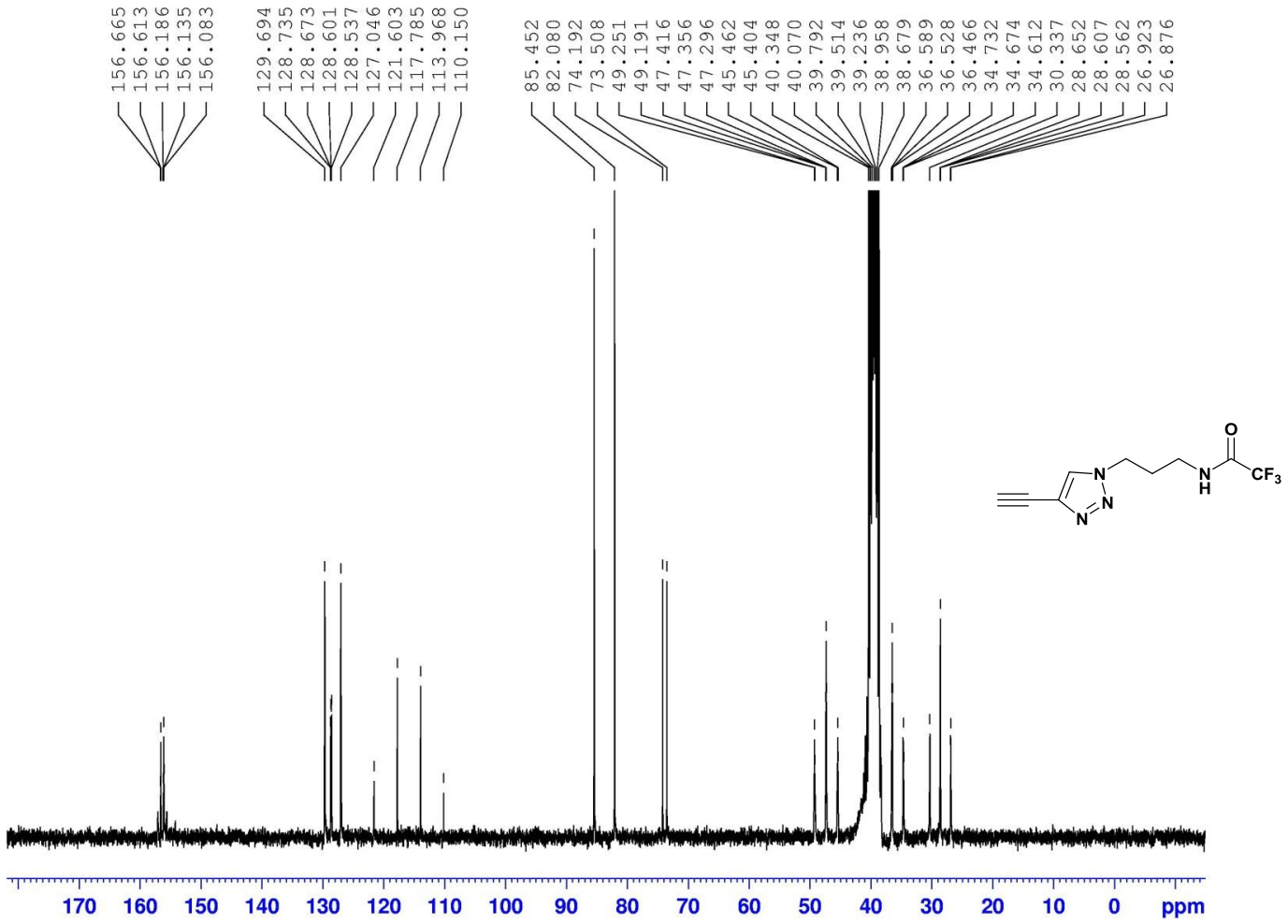

Figure S16. ^{1}H-^{13}C-gated decoupled spectrum of *N*-(3-(4-ethynyl-1*H*-1,2,3-triazol-1-yl)propyl)-2,2,2-trifluoroacetamide (**13**).

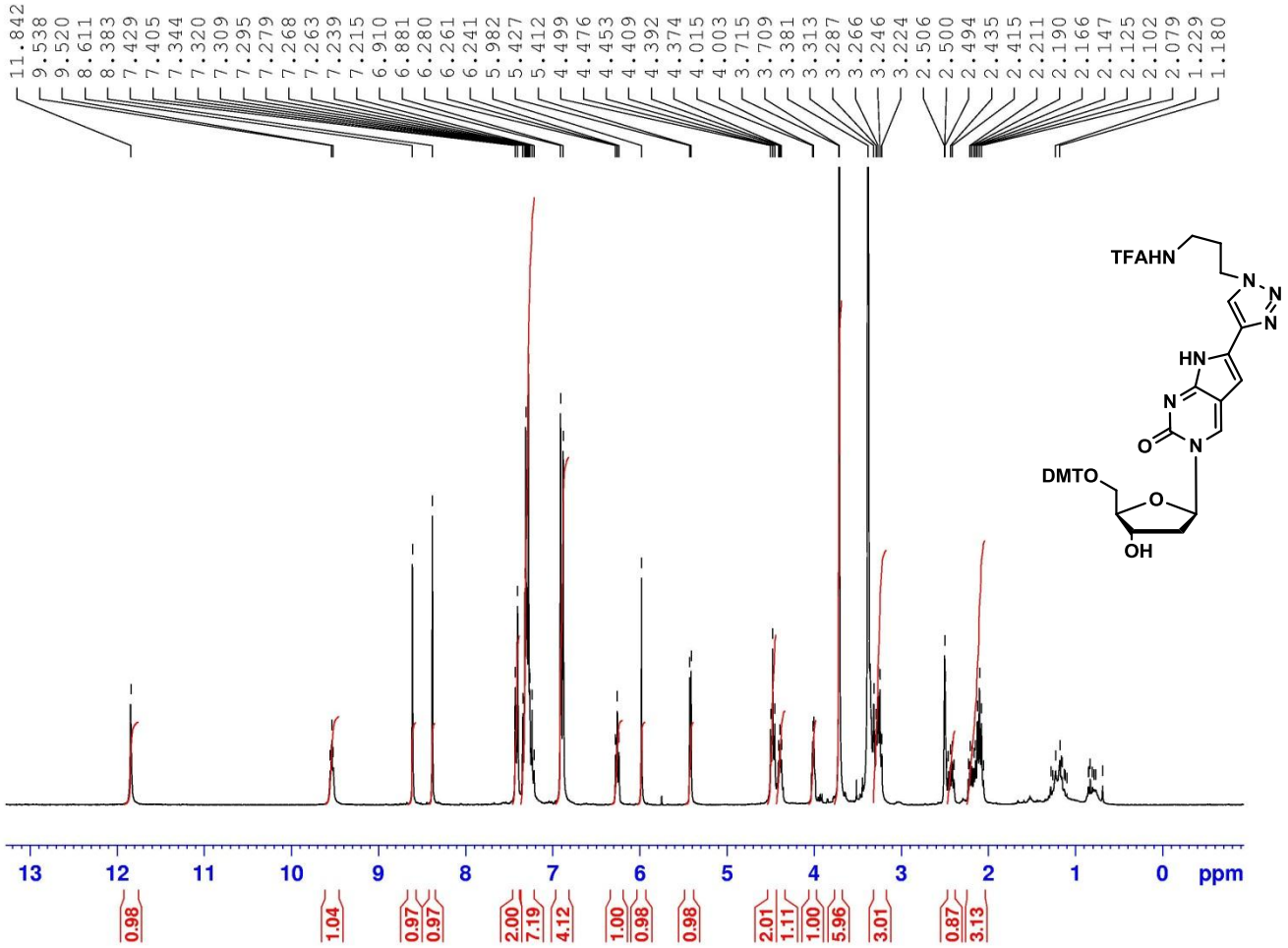

Figure S17. ^{1}H-NMR spectrum of trifluoroacetamide protected pyrrolo-dC analogue with DMT (**15**).

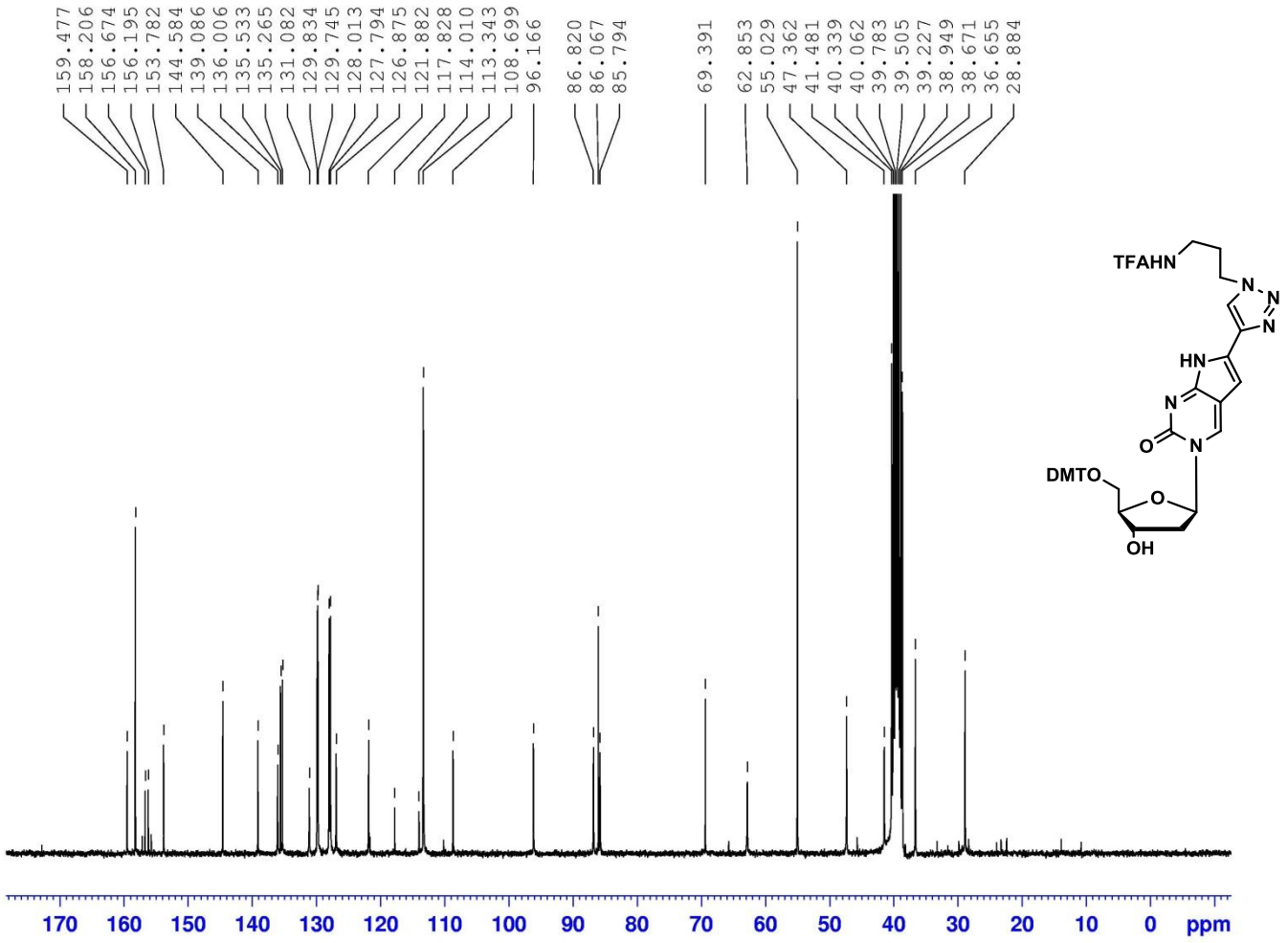

Figure S18. ^{13}C-NMR spectrum of trifluoroacetamide protected pyrrolo-dC analogue with DMT (**15**).

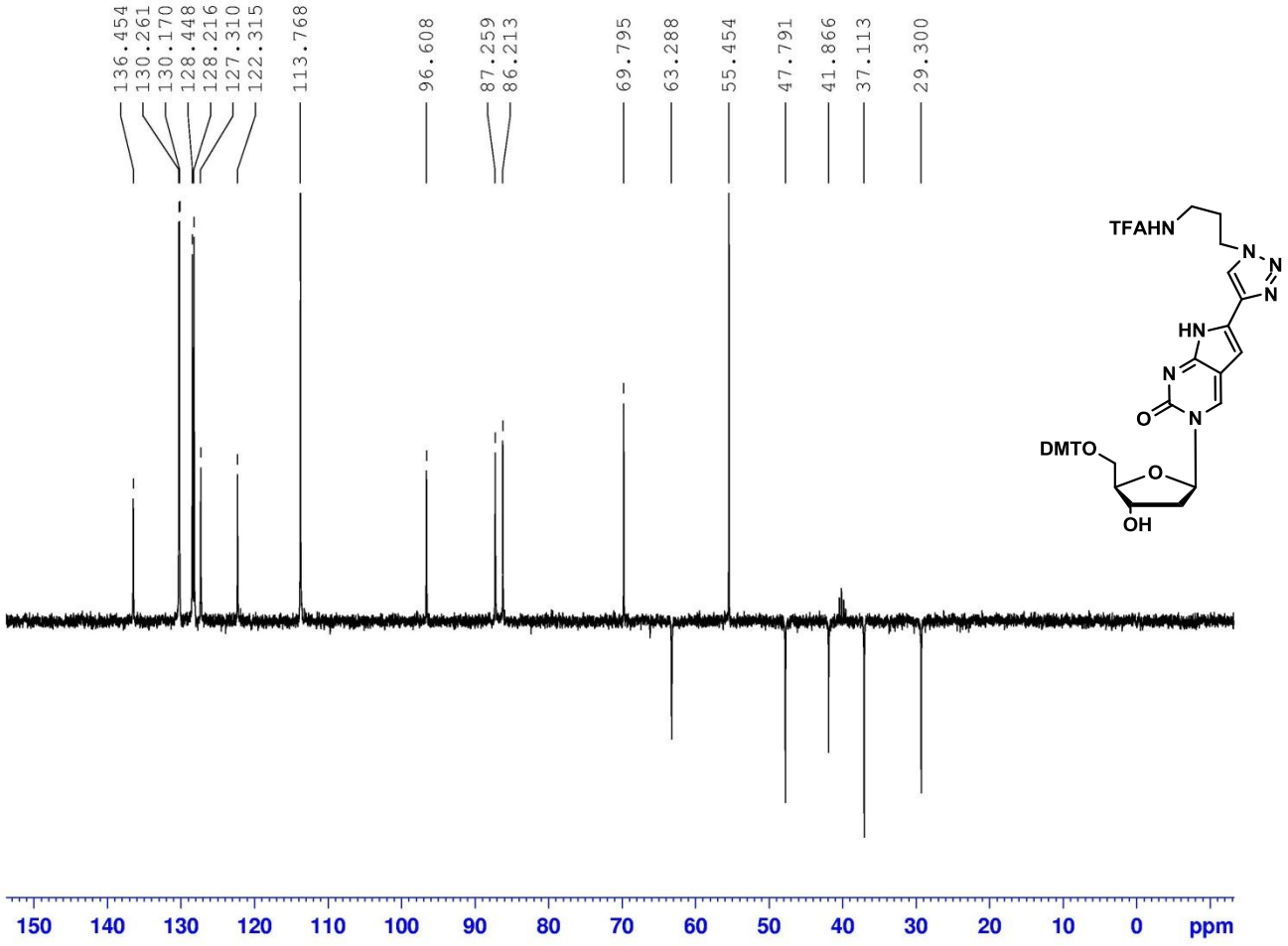

Figure S19. DEPT-135 spectrum of trifluoroacetamide protected pyrrolo-dC analogue with DMT (**15**).

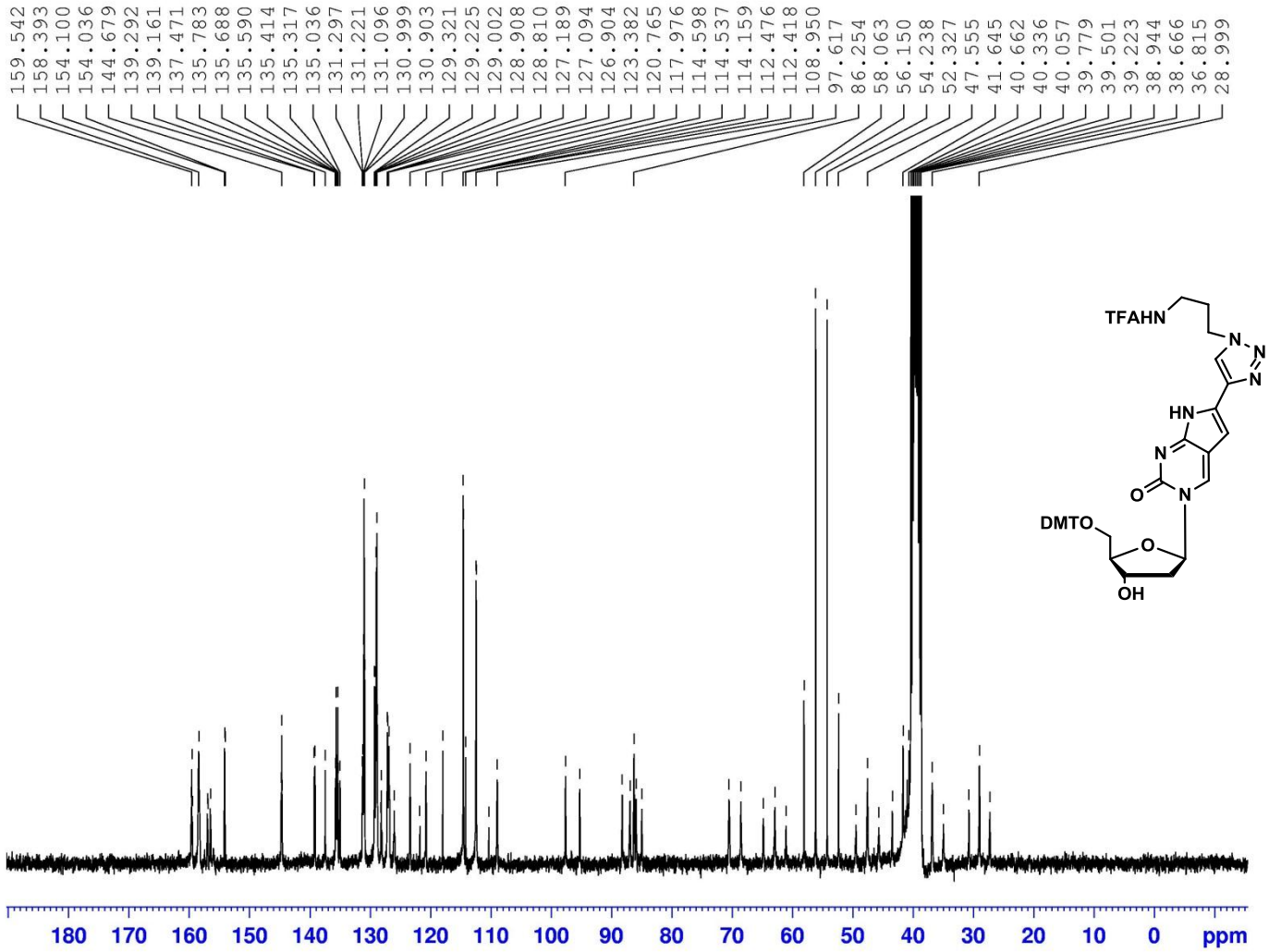

Figure S20. ^{1}H-^{13}C-gated decoupled spectrum of trifluoroacetamide protected pyrrolo-dC analogue with DMT (**15**).

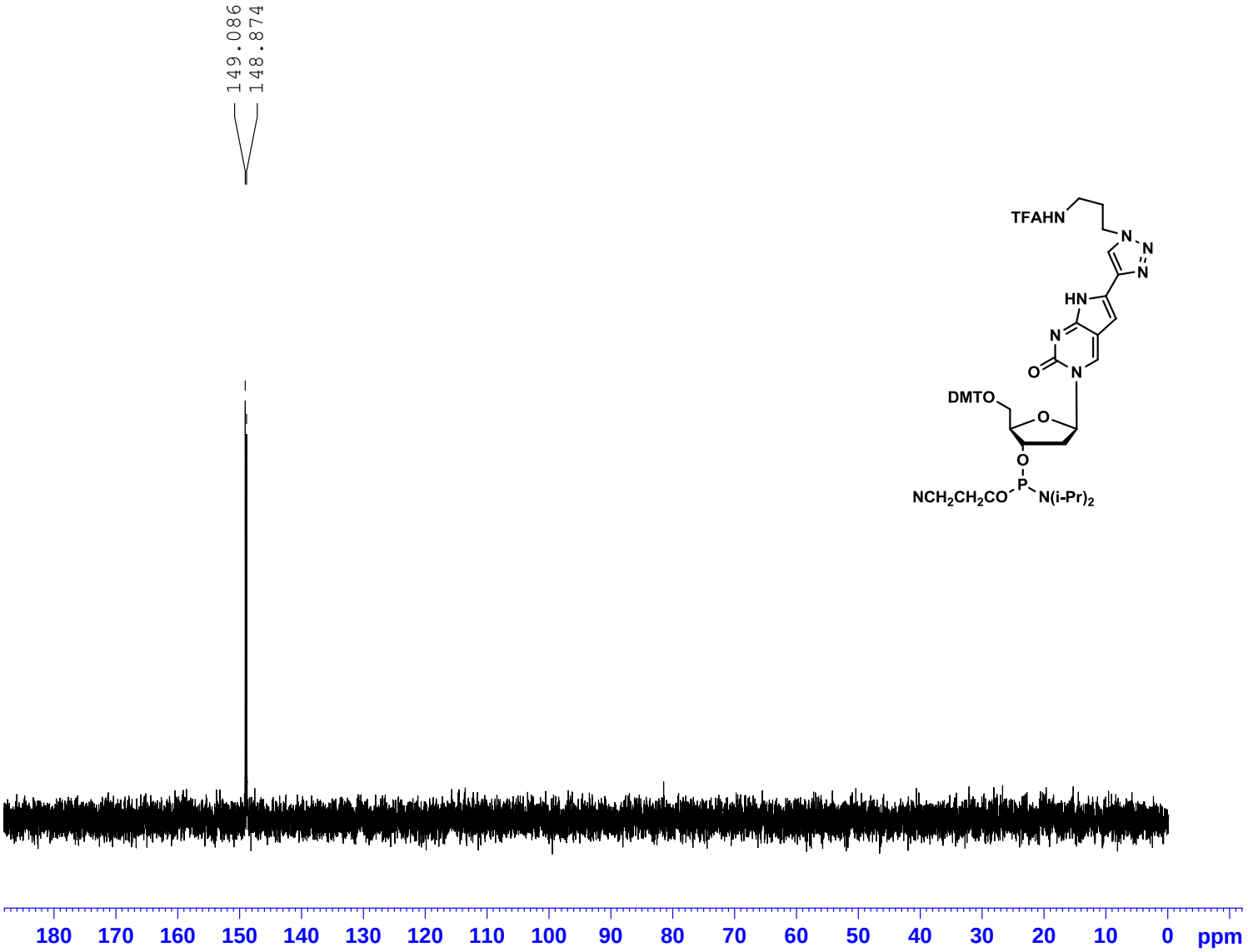

Figure S21. ^{31}P-NMR spectrum of phosphoramidite **5**.

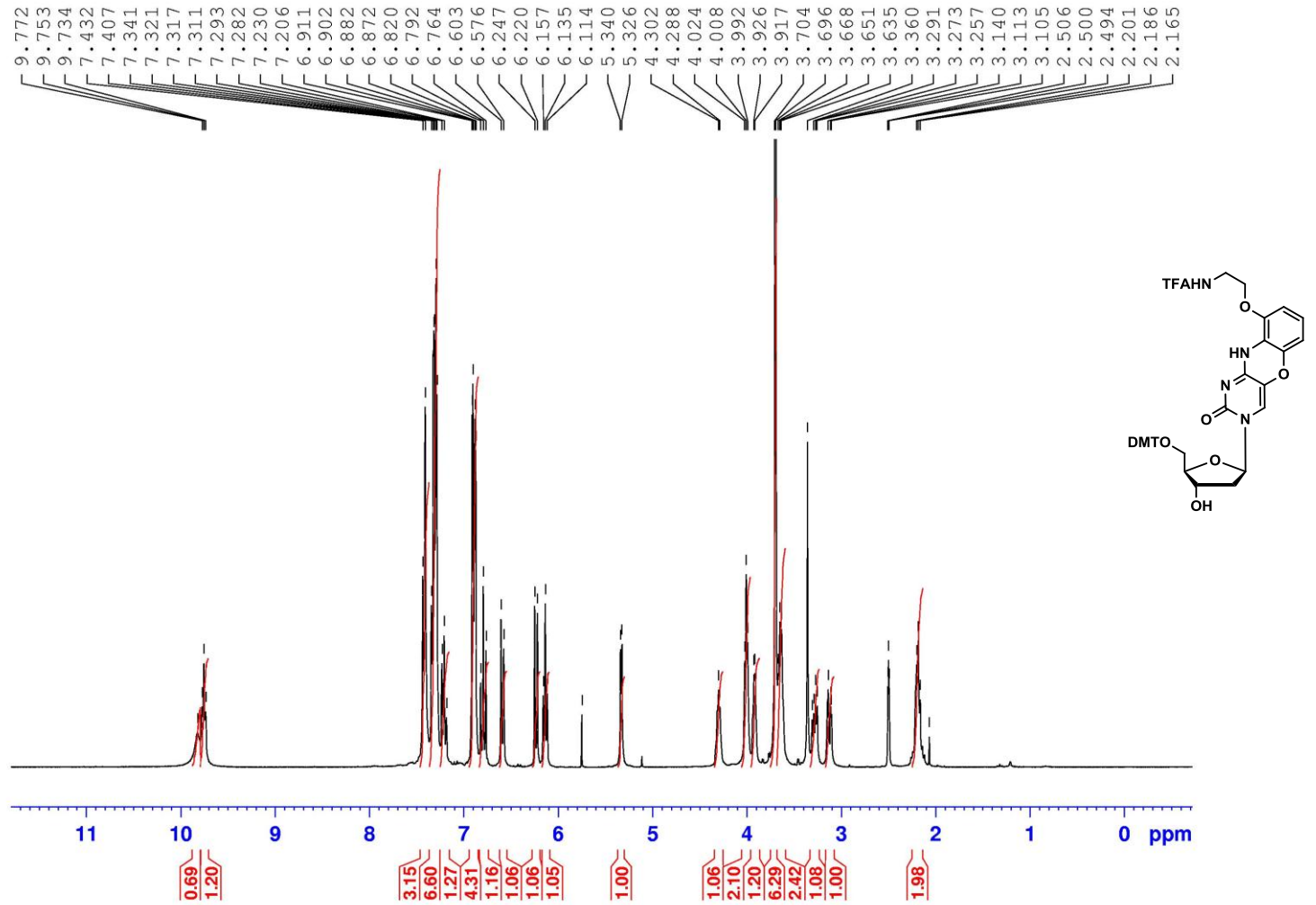

Figure S22. ^{1}H-NMR spectrum of the DMT-protected G-clamp.

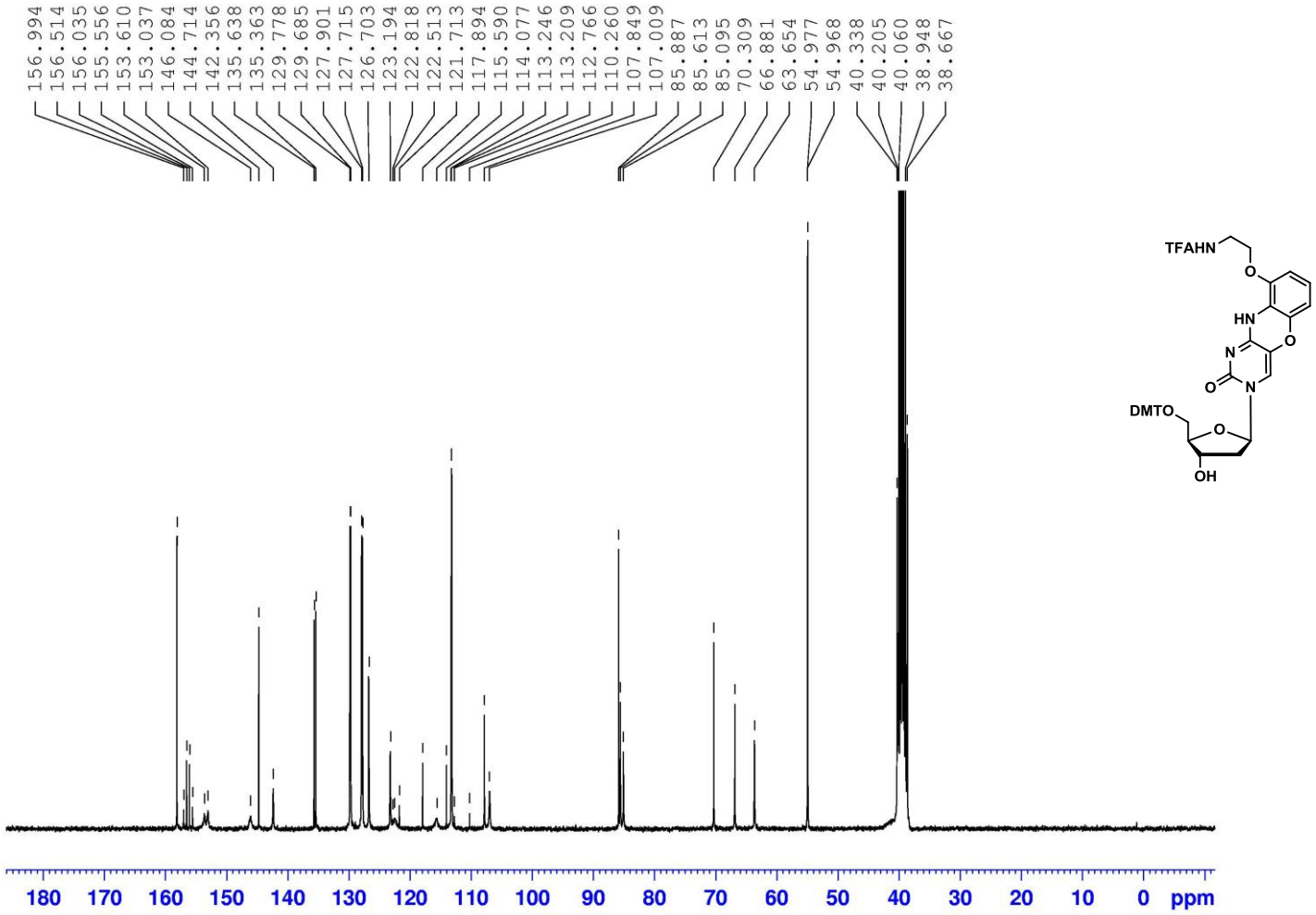

Figure S23. ^{13}C-NMR spectrum of the DMT-protected G-clamp.

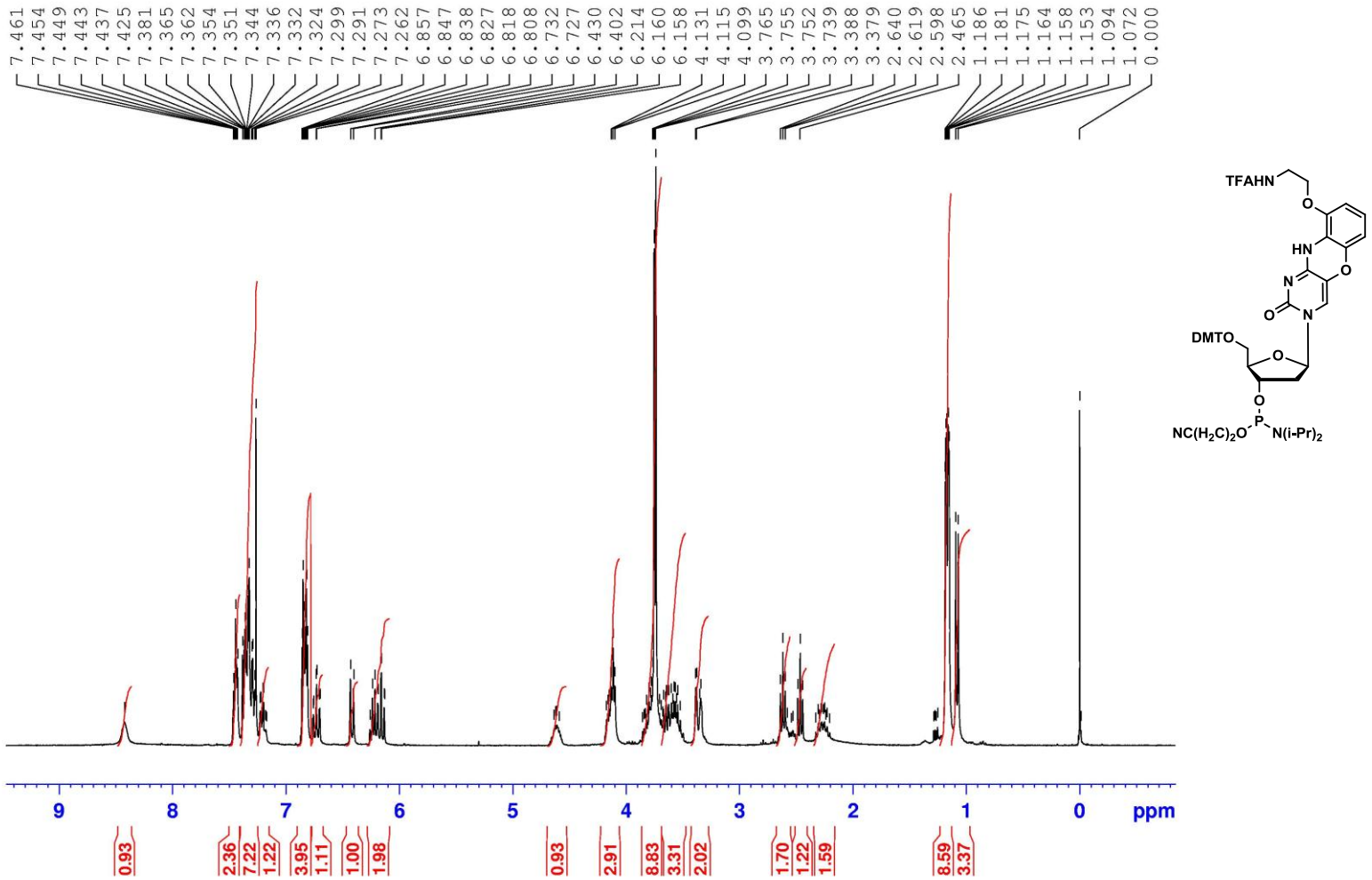

Figure S24. ^{1}H-NMR spectrum of phosphoramidite **16**.

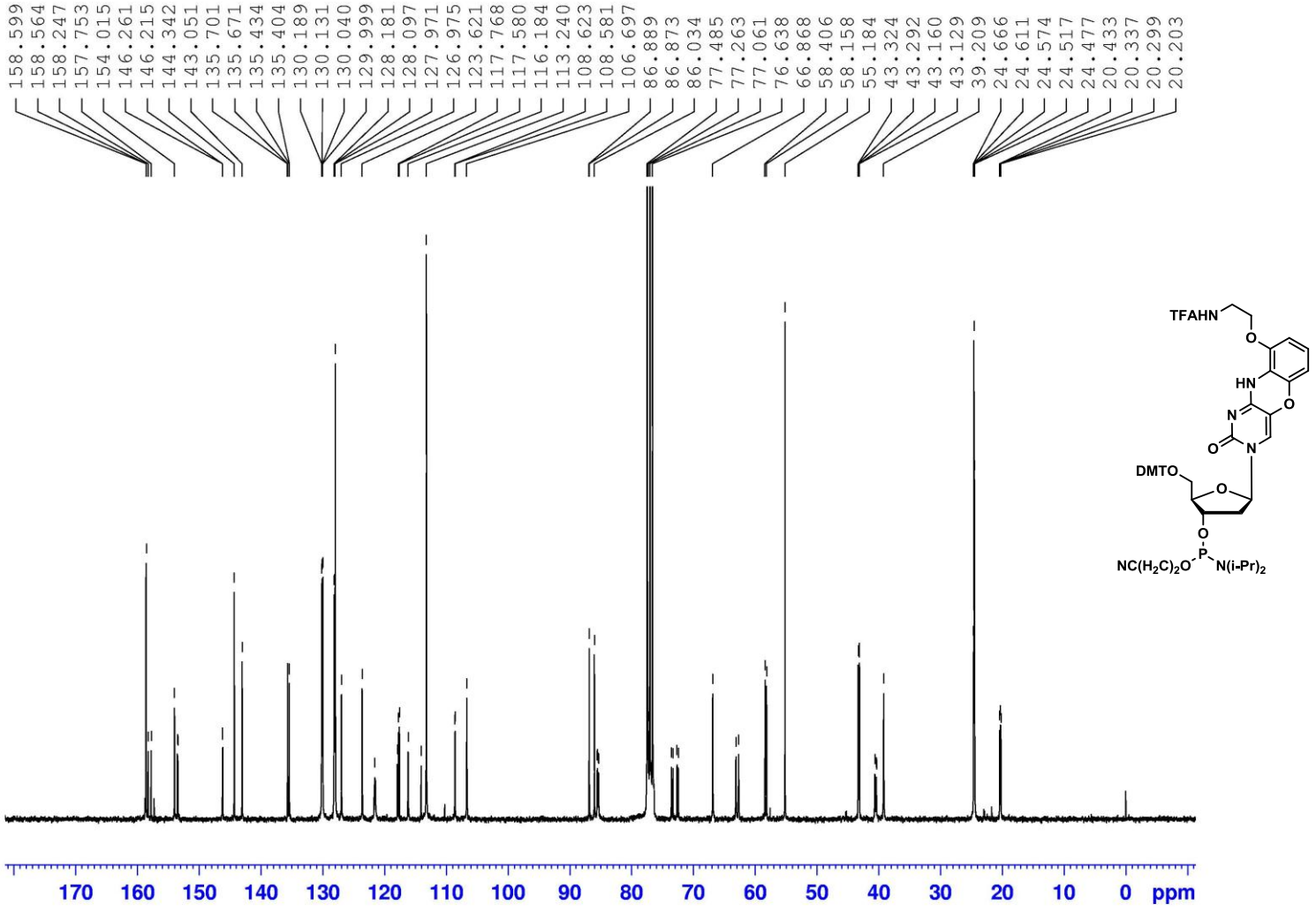

Figure S25. ^{13}C-NMR spectrum of phosphoramidite **16**.

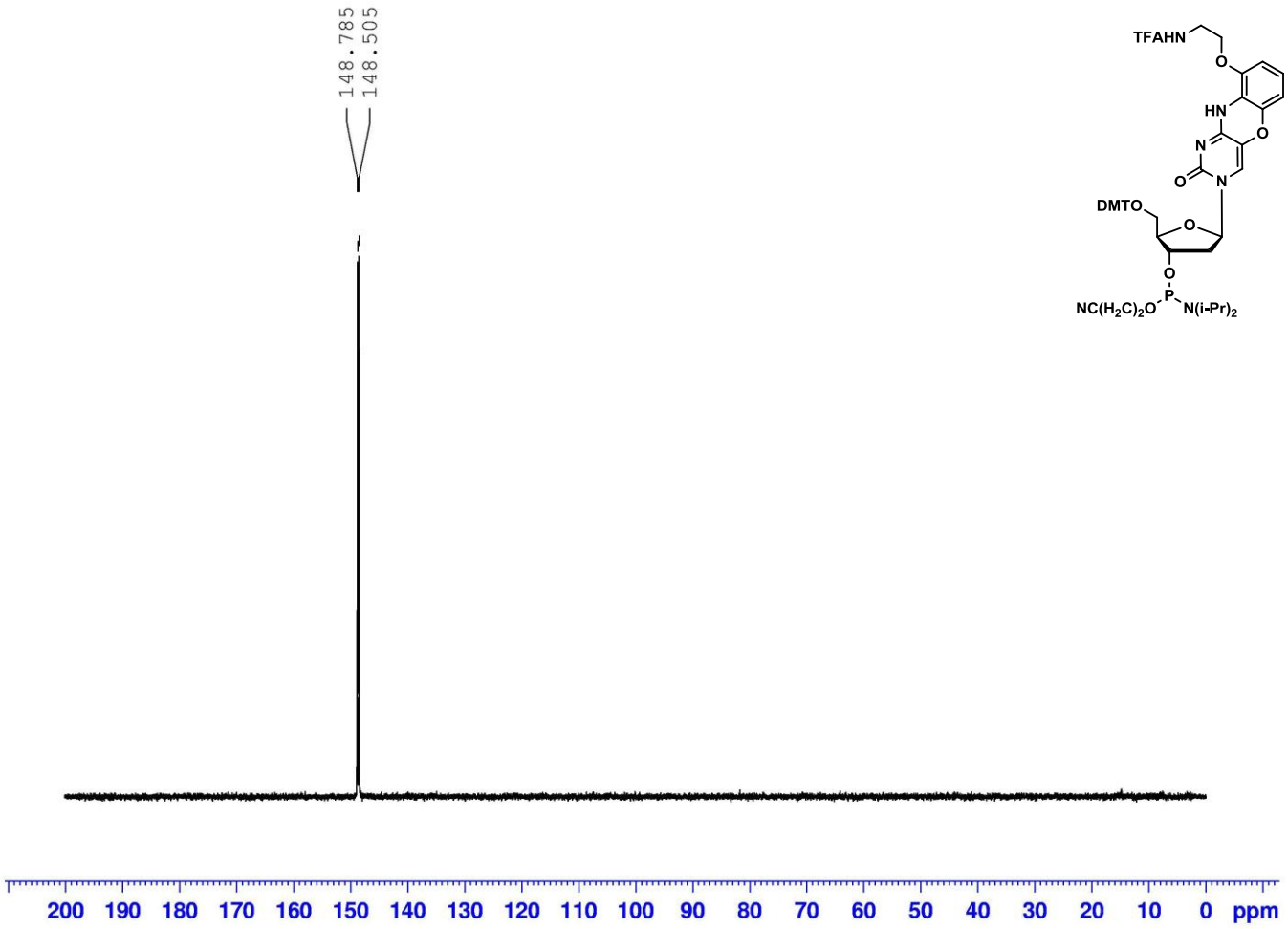

Figure S26. ^{31}P-NMR spectrum of phosphoramidite **16**.