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Data Article

Data for isolation and properties analysis of diastereomers of a mono-substituted phosphoryl guanine trideoxyribonucleotide



Alexander A. Lomzov^{a, c, *}, Maxim S. Kupryushkin^a,
 Andrey V. Shernyukov^{b, c}, Mikhail D. Nekrasov^a,
 Ilya S. Dovydenko^a, Dmitry A. Stetsenko^{a, c},
 Dmitrii V. Pyshnyi^{a, c, **}

^a Institute of Chemical Biology and Fundamental Medicine, SB RAS, 8 Lavrentiev Avenue, Novosibirsk, 630090, Russia

^b N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, SB RAS, 9 Lavrentiev Avenue, Novosibirsk, 630090, Russia

^c Novosibirsk State University, 2 Pirogova St., Novosibirsk 630090, Russia

ARTICLE INFO

Article history:

Received 12 April 2019

Received in revised form 23 May 2019

Accepted 4 June 2019

Available online 20 June 2019

Keywords:

Phosphoryl guanine oligonucleotide
 RP-HPLC

Circular dichroism
 NMR

Molecular dynamics
 Diastereomer assignment phosphodiesterase digestion assay
 Spatial structure

ABSTRACT

This article presents new data on the properties of the diastereomers of a mono-substituted phosphoryl guanine trideoxyribonucleotides d(TpCp*A) [1,2]. The data include information on isolation, identification, treatment with snake venom phosphodiesterase and structural analysis by 1D and 2D NMR spectroscopy and restrained molecular dynamics analysis. The data can be used for preparation, analysis, application of phosphoryl guanine oligonucleotide and for development of new nucleic acids derivatives. This data article is associated with the manuscript titled "Diastereomers of a mono-substituted phosphoryl guanine trideoxyribonucleotide: isolation and properties" [1].

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DOI of original article: <https://doi.org/10.1016/j.bbrc.2019.04.024>.

* Corresponding author.

** Corresponding author.

E-mail addresses: lomzov@niboch.nsc.ru (A.A. Lomzov), pyshnyi@niboch.nsc.ru (D.V. Pyshnyi).

<https://doi.org/10.1016/j.dib.2019.104148>

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Specifications Table

Subject area	Chemistry, Physical Chemistry, Biology
More specific subject area	Biochemistry and physical chemistry of nucleic acids
Type of data	Table, graph, figure
How data was acquired	High pressure liquid chromatography, mass spectroscopy, Circular Dichroism spectroscopy, 1D and 2D NMR, Molecular dynamics simulations
Data format	Raw and analyzed data
Experimental factors	Native trinucleotide d(TpCpA) and individual diastereomers of mono-substituted phosphoryl guanine oligonucleotide d(TpCp*A) were purified and analyzed
Experimental features	Individual diastereomers of mono-substituted phosphoryl guanine oligonucleotide d(TpCp*A) were purified by RP-HPLC using C18 sorbent and gradient of acetonitrile. MALDI-TOF MS analysis was conducted on Reflex III, Autoflex Speed with 3-hydroxypicolinic acid as a matrix. Temperature series of CD spectra were measured on a J-600 spectropolarimeter. NMR spectra were acquired on a Bruker Avance 600 MHz spectrometer. MD simulation was performed using AMBER 14 MD modeling software with GPU accelerated code
Data source location	Institute of Chemical Biology and Fundamental Medicine of Siberian Branch of the Russian Academy of Sciences, 8 Lavrentiev Ave., Novosibirsk, 630090, Russian Federation NMR data were collected in N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry of Siberian Branch of the Russian Academy of Sciences, 9 Lavrentiev Ave., Novosibirsk, 630090, Russian Federation
Data accessibility	Data is with this article
Related research article	A. A. Lomzov, M. S. Kupryushkin, A. V. Shernyukov, M. D. Nekrasov, I. S. Dovydenko, D. A. Stetsenko, D. V. Pyshnyi, Diastereomers of a mono-substituted phosphoryl guanine trideoxyribonucleotide: Isolation and properties, Biochem. Biophys. Res. Commun., 514, 2019, 807–811 [1].

Value of the data
• Data on the isolation, SVPDE digestion and identification of the mono-substituted phosphoryl guanine oligonucleotide d(TpCp*A) diastereomers can be helpful for other researchers to analyze phosphate modified nucleic acids derivatives • The data can be used by other researchers with an interest in synthesis, purification and application of nucleic acid derivative and analogues • Our data contribute to the properties of phosphate-substituted oligonucleotides • This data could be useful for the researchers with an interest in biosensor development and biomedical application of nucleic acids

1. Data

Data reported here describe the features of diastereomers of a trideoxynucleotide 5'-TpCpA-3' modified at the phosphate group near the 3'-end with a single 1,1,3,3-tetramethyl guanidine group revealed from studies by Reverse phase HPLC (RP-HPLC) separation and analysis, SVPDE digestion, circular dichroism spectroscopy, 1D and 2D NMR analysis and restrained molecular dynamics simulation.

1.1. RP-HPLC analysis of oligonucleotides reaction mixture after synthesis

Reverse phase HPLC analysis of oligonucleotides were performed for reaction mixture of native d(TpCp*A) and mono-substituted phosphoryl guanine (PG) oligonucleotides d(TpCp*A) after synthesis. Analytical and preparative chromatograms are shown in Fig. 1.

MALDI-TOF MS spectra of oligonucleotides.

Matrix-assisted laser desorption ionization – time of flight mass spectroscopy (MALDI-TOF MS) was conducted for the isolated by RP-HPLC samples of d(TpCpA) and diastereomers of d(TpCp*A) (Fig. 2).

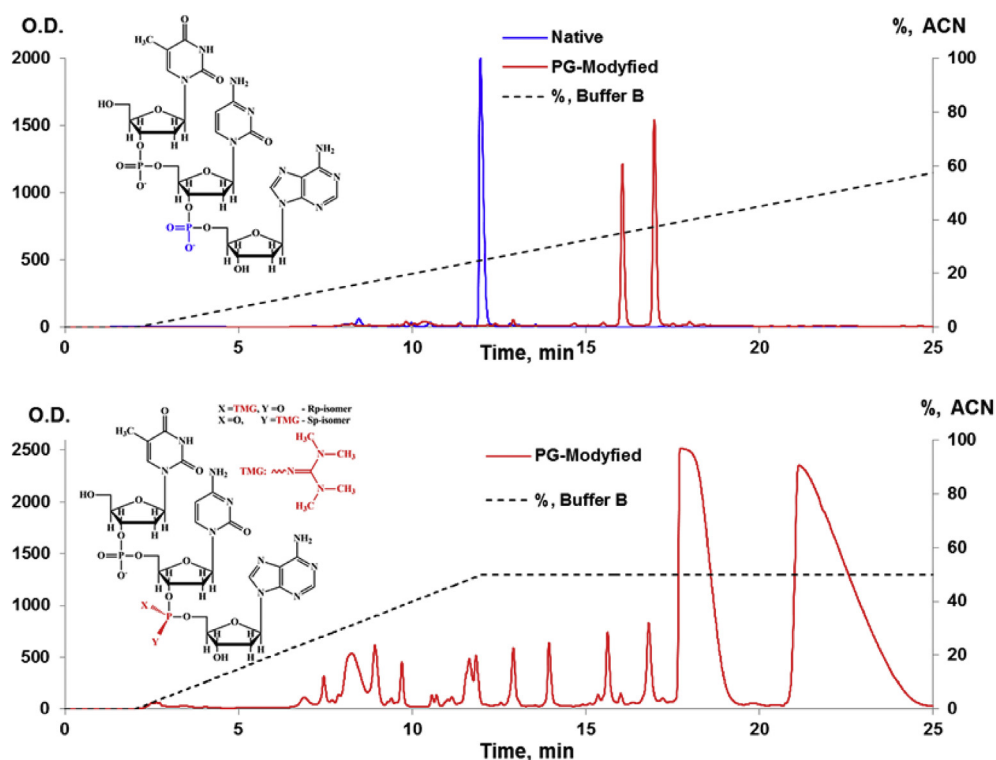


Fig. 1. RP-HPLC analysis of reaction mixtures of native TpCpA (blue) and modified TpC*pA (red, * - position of modified phosphate) deoxyribonucleotides reaction mixture after detritilation. Upper chromatographic profiles are analytical and lower is preparative. Details of experiments see in section Material and methods.

1.2. RP-HPLC profiles of oligonucleotides after SVPDE digestion

We treated native and mono-substituted oligonucleotides with snake venom phosphodiesterase (SVPDE) for 150 h. Three oligomers after digestion by SVPDE were analyzed by RP-HPLC (Fig. 3).

1.3. Circular dichroism spectra of oligonucleotides at high and low temperatures

Circular dichroism spectra were used for characterisation structure of native and modified oligonucleotides at low (25 °C) and high (95 °C) temperatures (Fig. 4).

1.4. NMR spectroscopy analysis of oligonucleotides

1D and 2D NMR spectroscopy experiments were performed for isolated mono-substituted phosphoryl guanidine oligonucleotides d(TpCp*A) and their mixture (Figs. 5–9, Tables 1–10).

Assignment of the NMR signals.

1.5. Molecular dynamics simulation data analysis

Molecular dynamics simulation with the NOESY NMR restraints were performed for diastereomers of d(TpCp*A). The NOESY NMR restraints for two mixing times (0.4 and 0.8 s) and restraint penalties calculates as an average of last frames of every annealing cycle are shown were collected (Tables 11–15,

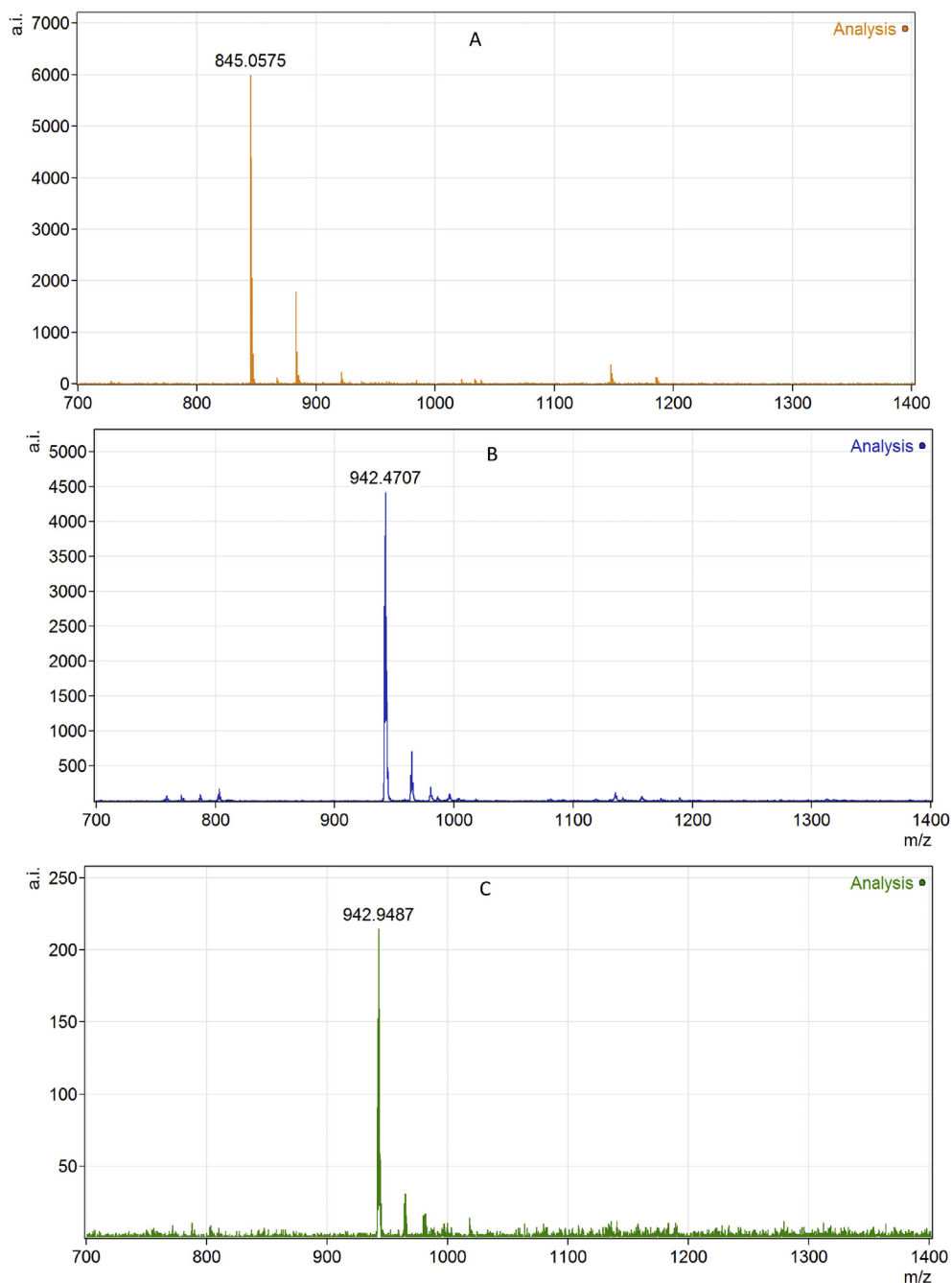


Fig. 2. MALDI-TOF MS spectra of native (A) and PG-modified 'fast' (B) and 'slow' (C) trinucleotides.

Figs. 12–14). The data on cluster analysis of the MD trajectories are shown in Tables 16–19. Molecular structures of the trinucleotides most represented in the MD simulation can be found in the Supplementary Data of this article. The structures flexibility was analyzed using RMSD map for the oligonucleotides structures after simulation annealing (Fig. 10 and Fig. 11).

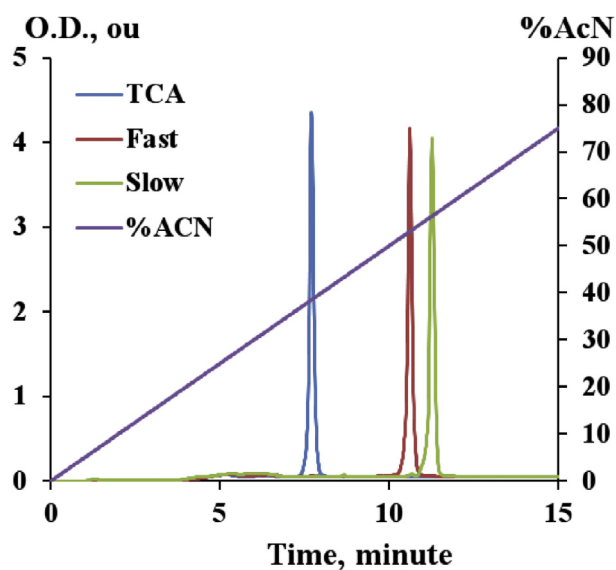


Fig. 3. RP-HPLC profiles of TpCpA, TpCp*A('fast') and TpCp*A('slow') before SVDP digestion. Data on oligonucleotide analysis after digestion shown in Fig. 2 in Ref. [1].

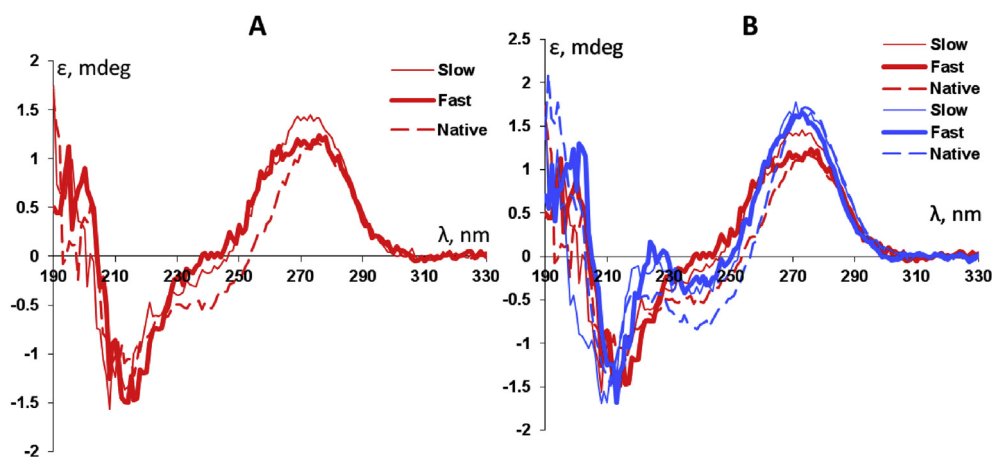


Fig. 4. Circular dichroism spectra of native (dashed line), 'fast' (thick line) and 'slow' (thin line) trinucleotides at 95 °C (A) and comparison with 25 °C (B).

2. Experimental design, materials and methods

2.1. Synthesis

Standard phosphoramidite solid-phase synthesis of all modified and unmodified oligonucleotides containing phosphodiester linkages (PO) was carried out on an ASM-800 DNA/RNA synthesizer ("Biosset", Russia). Oligonucleotides were synthesized at 1 μ mol scale, using standard commercial 2-

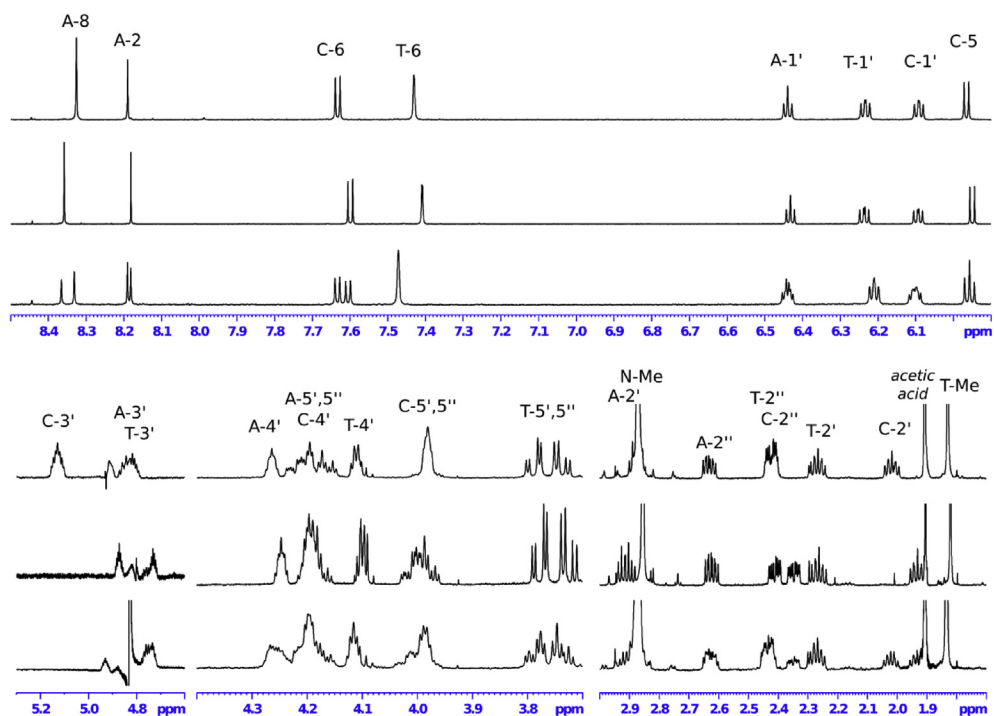


Fig. 5. Fragments ^1H NMR spectra (600 MHz, D_2O). For each fragment 'slow' (top), 'fast' (middle) and their 1:1 mixture (down).

cynoethyl deoxynucleoside phosphoramidites and CPG solid supports (Glen Research, USA). Oligonucleotides with internucleotide tetramethyl phosphoryl guanidine group was synthesized as described in Refs. [2,3].

2.2. HPLC analysis and separation

Native and modified oligonucleotides were isolated by reverse-phased HPLC on an Agilent 1200 HPLC system (USA) using a Zorbax SB-C18 5 mm column 4.6×150 mm. For native oligonucleotide linear gradient of buffer B (acetonitrile 0–50% in 20 mM triethylammonium acetate, pH 7.0), a flow rate of 2 ml min $^{-1}$ was used. For separation of diastereomers complex gradient of buffer B (20% acetonitrile in 20 mM triethylammonium acetate, pH 7.0) according to Fig. 1 was used.

Fractions containing the appropriate peak were evaporated in vacuo, the bulk of triethylammonium acetate was removed by repeated coevaporations with ethanol. After evaporated until dryness oligonucleotides were dissolved in deionized water and stored at -20°C . Absorption spectra were recorded at wavelengths from 220 to 600 nm.

2.3. MALDI-TOF MS analysis

Matrix-assisted laser desorption ionization – time of flight mass spectroscopy (MALDI-TOF MS) was conducted on Reflex III, Autoflex Speed (Bruker, Germany) with 3-hydroxypicolinic acid as a matrix with positive ion detection scan mode.

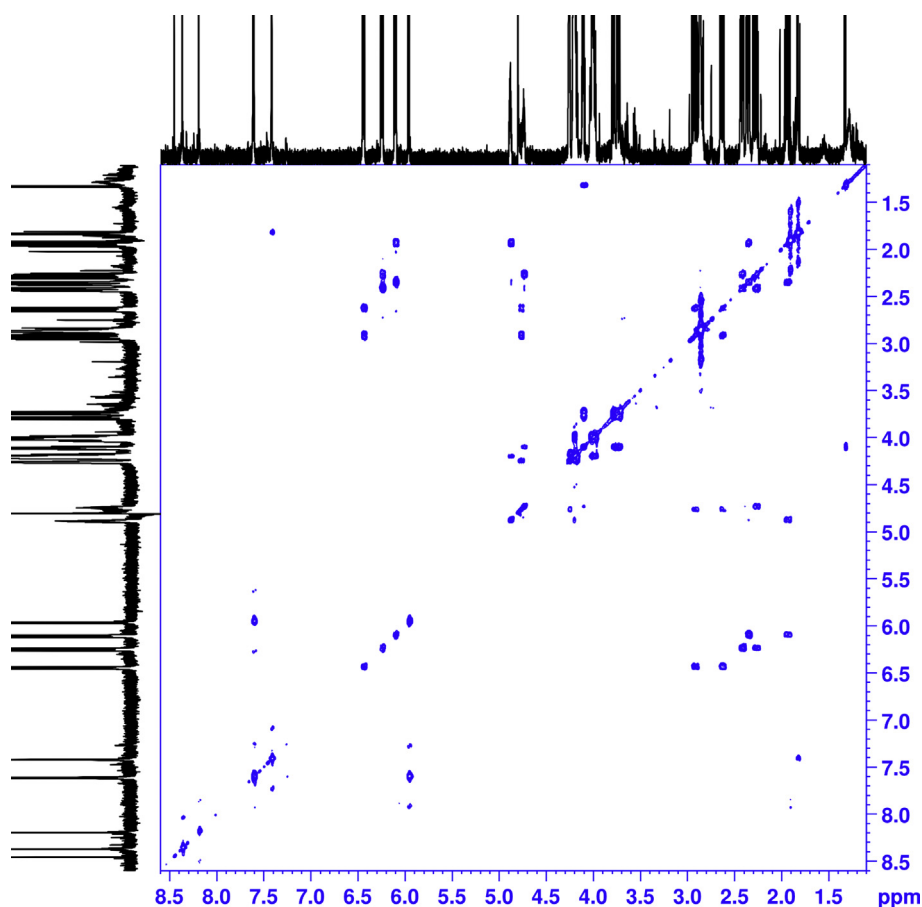


Fig. 6. ^1H – ^1H COSY NMR spectra of the 'fast' isomer.

2.4. SVDPE digestion assay

Oligonucleotides were incubated with SVDPE at 37 °C. Reaction mixture contained 3 μg of SVDPE, 20 mM Tris-HCl, pH 9.0, 5 mM MgCl_2 and 0.1 mM oligonucleotide [4]. Aliquots of 20 μl withdrawn at 0.5, 1, 24, 48 and 150h, heated to 65 °C for 30 min, then analyzed by RP-HPLC.

2.5. Circular dichroism (CD) experiments

CD spectra were measured on a J-600 spectropolarimeter (Jasco, Japan) using temperature-controlled 1 mm pathlength quartz cell. The measurements were performed in the range 190–330 nm at 25 °C and 95 °C. CD curves were recorded every 1 nm, bandwidth 2 nm and averaged over 5 scans. Oligonucleotides in concentration of 0.1 mM in milliQ water were used.

2.6. Ultraviolet (UV) spectra

UV spectra were recorded using 1 mL quartz cell with pathlength 1 cm on a UV-2100 spectrophotometer (Shimadzu, Japan). The measurements were performed in the range 190–330 nm at 25 °C.



Concentration of trinuclotides were determined from their UV absorbance using calculated molar extinction coefficients at 260 nm [5].

All the spectra were acquired on a Bruker Avance 600 MHz spectrometer. The chemical shifts in NMR spectra were calibrated relative to DSS by substitution referencing [6]. The 1D and 2D experiments were performed at 25 °C for assignments and included ^1H , $^1\text{H}\{^31\text{P}\}$, $^{13}\text{C}\{^1\text{H}\}$, ^{31}P , $^{31}\text{P}\{^1\text{H}\}$, $^1\text{H} \times ^1\text{H}$ COSY, $^1\text{H} \times ^{13}\text{C}$ HMB, $^1\text{H} \times ^{31}\text{P}$ HMB, $^1\text{H} \times ^1\text{H}$ TOCSY, ^1H DOSY, $^1\text{H} \times ^1\text{H}$ NOESY (with mixing time 0.25 s), $^1\text{H} \times ^1\text{H}$ ROESY (with mixing time 0.25 s). Spectra were processed on Bruker Topspin and analyzed in CCPNMR2 [7]. The assignments of signals in the spectra were carried out by their combined analysis. The spin systems of deoxyribose residues were identified from ^1H – ^1H COSY (Figs. 6–7) and ^1H – ^1H TOCSY spectra. The diastereotope assignment of the signals of proton H2' and H2'' were carried out on the basis of ^1H – ^1H NOESY spectra (see Figs. 8 and 9) and by comparison with published chemical shift ranges [8].

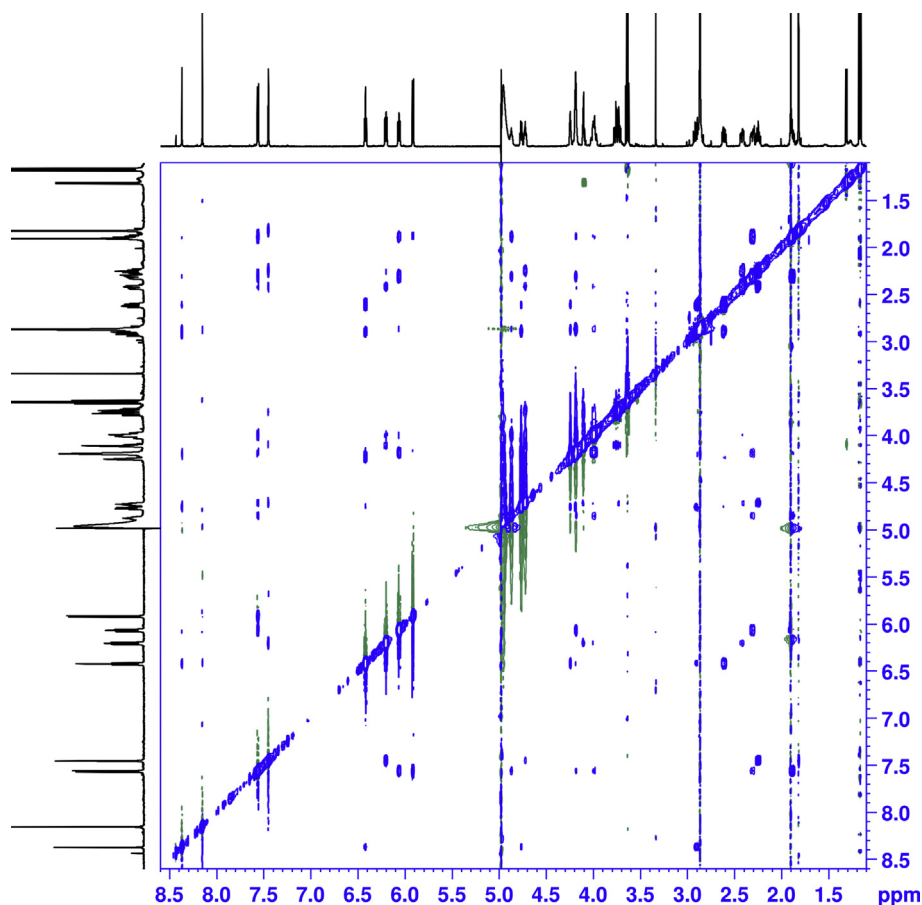


Fig. 8. ^1H – ^1H NOESY NMR (mixing time 0.8s, $T = 8.0^\circ\text{C}$) spectra of the 'fast' isomer.

Distance restraints were derived from NOESY cross-peak intensities from spectra recorded at 8°C with mixing times 0.4 s and 0.8 s correspondingly. The fixed cytosine H5–H6 distance (2.5 Å) was used as internal reference to determine the quality of the calibration.

After the assignment of the signals in the 2D -spectra (the results are shown in Tables S1–10), the spin-spin interaction constants 1H – 1H were extracted from the 1H { $^{31}\text{P}}$ spectra and then the obtained data were used to measure the 1H – ^{31}P constants from the 1H spectra.

2.8. Molecular dynamics simulations

The molecular dynamics (MD) simulations were performed using Amber 14 software [9]. Structures of TpCp*A were generated using xleap program (AmberTools 14) based on B-form DNA geometry. Particular atoms charges of modified nucleotides were calculated using RESP method based on structures optimized by Hartree-Fock method and 6-31G* basis in Gaussian'09 software [10]. Then the library files for Rp- and Sp-isomers of tetramethyl phophorylguanine of 3'-adenosine were generated. NMR distance restraints were used for subsequent refinement of the structure. The upper bounds of the restraints were set to +0.5 Å of the calculated NOE distance. The lower bounds of the restraints were set 1.8 Å. Structural calculations were performed using the sander module of Amber 14 as described in Ref. [11]. The generalized Born implicit solvent model with the equivalent of 0.1 M 1–1

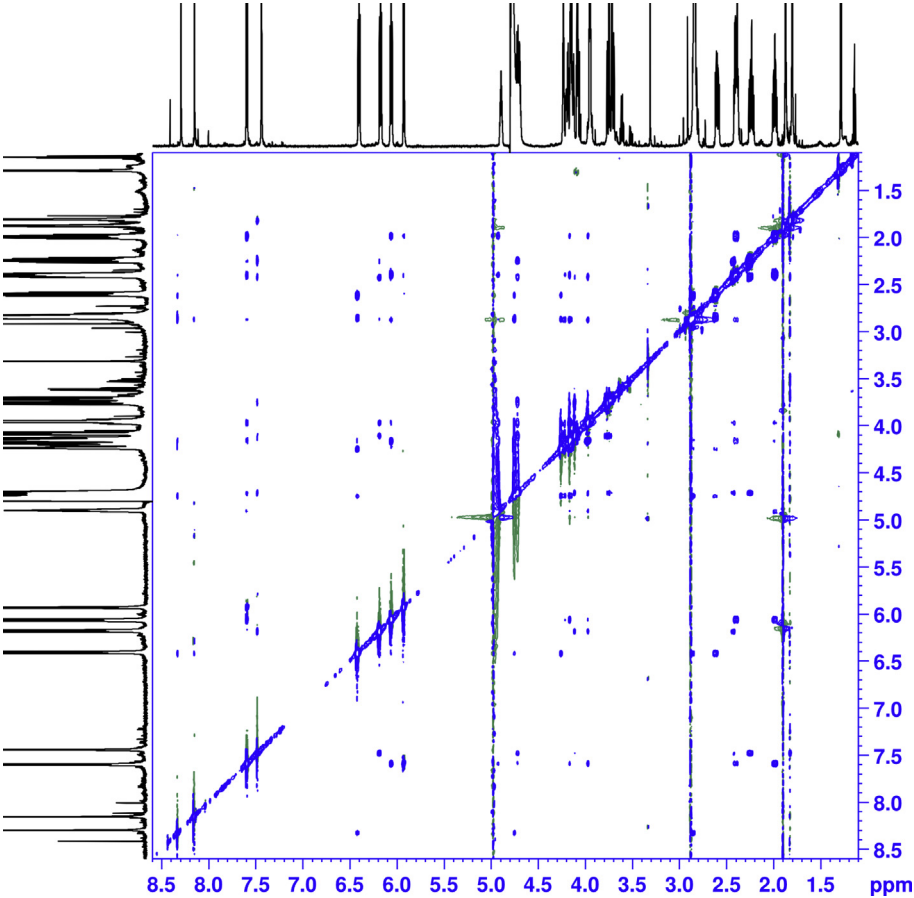


Fig. 9. ^1H - ^1H NOESY NMR (mixing time 0.8s, T = 8.0 °C) spectra of the 'slow' isomer.

Table 1

Chemical shifts of 'fast' diastereomer, ppm.

	dT	dC	d(p*A)
H1'	6.25	6.10	6.44
H2	—	—	8.19
H2'	2.27	1.93	2.91
H2''	2.42	2.36	2.62
H3'	4.74	4.88	4.77
H4'	4.11	4.22	4.27
H5	—	5.96	—
H5' & H5''	3.79 и 3.73	4.04 и 4.00	4.18 и 4.20
H6	7.42	7.61	—
H7	1.83	—	—
H8	—	—	8.37
C1'	88.18	88.34	86.21
C2	161.56	159.84	155.53
C2'	40.24	40.48	41.20
C3'	78.12	78.55	73.09
C4	178.63	168.61	151.56
C4'	87.96	86.50	87.79
C5	114.49	99.16	121.36
C5'	63.96	67.43	68.20
C6	139.19	143.75	158.17
C7	15.50	—	—
C8	—	—	142.49
(CH ₃) ₂ -N-CN-Cp*A	2.86		
(CH ₃) ₂ -N-CN-Cp*A	42.38		
-C=N-Cp*A	165.88		
TpC	-0.82		
Cp*A	0.37		

Table 2Coupling constants³¹P–¹³C of 'fast' diastereomer, Hz.

	dT	dC		d(p*A)
	TpC	TpC	Cp*A	Cp*A
C2'	2.9	0	2.9	0
C3'	5.3	0	5.5	0
C4'	6.8	8.8	7.6	8.8
C5'	0	5.5	0	6.8
C=N-Cp*A = 7.5				

ions, the weak-coupling algorithm of temperature regulation and integration time step of 0.001 ps were used. Simulation annealing protocol was applied and includes 100 cycles of heating to 800 K for 0.25 ns and following cooling to 300 K for 0.25 ns. Force constant 1 kcal/[mol·Å²] for distance restraints was applied.

Trajectory analysis was performed using the cpptraj tool of Amber 16 [12]. Hierarchical cluster analysis was conducted for final structures of simulation annealing. Molecular graphics were prepared with the UCSF Chimera package [13]. Hierarchical cluster analysis was used for productive MD trajectory analysis of the DNA duplexes without terminal base pairs. The random sieve of 100 was applied.

Table 3
Chemical shifts of 'slow' diastereomer, ppm.

	dT	dC	d(p*A)
H1'	6.23	6.09	6.44
H2	—	—	8.19
H2'	2.27	2.02	2.88
H2''	2.42	2.42	2.63
H3'	4.73	4.92	4.75
H4'	4.11	4.20	4.26
H5	—	5.96	—
H5' & H5''	3.74 и 3.79	3.98 и 3.99	4.17 и 4.22
H6	7.41	7.64	—
H7	1.82	—	—
H8	—	—	8.33
C1'	88.14	88.42	86.25
C2	160.69	159.89	155.52
C2'	40.22	40.7	41.27
C3'	78.11	78.64	73.20
C4	177.5	168.65	151.56
C4'	88.02	86.40	87.82
C5	114.45	99.1	121.40
C5'	63.94	68.10	67.29
C6	139.29	143.84	158.2
C7	15.37	—	—
C8	—	—	142.40
(CH ₃) ₂ –N–CN–Cp*A	2.87		
(CH ₃) ₂ –N–CN–C*pA	42.42		
–C=N–Cp*A	165.91		
TpC	–0.89		
Cp*A	0.21		

Table 4
Coupling constants³¹P–¹³C of 'slow' diastereomer, Hz.

	dT	dC		d(p*A)
	TpC	TpC	Cp*A	Cp*A
C2'	2.8	0	2.6	0
C3'	5.4	0	6.5	0
C4'	6.6	8.5	6.9	8.9
C5'	0	5.1	0	5.8
C=N–Cp*A = 7.7				

Table 5
Coupling constants ¹H–¹H, ¹H–³¹P of adenosine monophosphate of 'fast' diastereomer, Hz.

	H1'	H2'	H2''	H3'	H4'	H5' & H5''	Cp*A
H1'	*	6.3	6.7	0	0	0	0
H2'	6.3	*	14.0	6.4	0	0	0
H2''	6.7	14.0	*	4.9	0	0	0
H3'	0	6.4	4.9	*	4.4	0	0
H4'	0	0	0	4.4	*	3.9	2.1
H5' & H5''	0	0	0	0	3.9	n.d..	n.d..
Cp*A	0	0	0	0	2.1	n.d..	*

Table 6Coupling constants $^1\text{H}-^1\text{H}$, $^1\text{H}-^{31}\text{P}$ of adenosine monophosphate of 'slow' diastereomer, Hz.

	H1'	H2'	H2''	H3'	H4'	H5' & H5''	Cp*A
H1'	*	6.5	6.5	0	0	0	0
H2'	6.5	*	14.0	6.4	0	0	0
H2''	6.5	14.0	*	4.8	0	0	0
H3'	0	6.4	4.8	*	4.3	0	0
H4'	0	0	0	4.3	*	3.9	2.1
H5' & H5''	0	0	0	0	3.9	11.5	4.9, 4.0
Cp*A	0	0	0	0	2.1	4.9, 4.0	*

Table 7Coupling constants $^1\text{H}-^1\text{H}$, $^1\text{H}-^{31}\text{P}$ of thymidine of 'fast' diastereomer, Hz.

	H1'	H2'	H2''	H3'	H4'	H5' & H5''	H6	H7	TpC
H1'	*	8.1	6.1	0	0	0	0	0	0
H2'	8.1	*	14.1	6.3	0	0	0	0	0
H2''	6.1	14.1	*	3.0	0	0	0	0	0
H3'	0	6.3	3.0	*	3.2	0	0	0	7.0
H4'	0	0	0	3.2	*	3.5	0	0	0
H5' & H5''	0	0	0	0	3.5	12.5	0	0	0
H6	0	0	0	0	0	0	*	1.1	0
H7	0	0	0	0	0	0	1.1	*	0
TpC	0	0	0	7.0	0	0	0	0	*

Table 8Coupling constants $^1\text{H}-^1\text{H}$, $^1\text{H}-^{31}\text{P}$ of thymidine of 'slow' diastereomer, Hz.

	H1'	H2'	H2''	H3'	H4'	H5' & H5''	H6	H7	TpC
H1'	*	8.0	6.1	0	0	0	0	0	0
H2'	8.0	*	14	6.2	0	0	0	0	0
H2''	6.1	14	*	3.0	0	0	0	0	0
H3'	0	6.2	3.0	*	3.2	0	0	0	7.0
H4'	0	0	0	3.2	*	3.5	0	0	0
H5' & H5''	0	0	0	0	3.5	12.5	0	0	0
H6	0	0	0	0	0	0	*	1.1	0
H7	0	0	0	0	0	0	1.1	*	0
TpC	0	0	0	7.0	0	0	0	0	*

Table 9Coupling constants $^1\text{H}-^1\text{H}$, $^1\text{H}-^{31}\text{P}$ of cytidine monophosphate of 'fast' diastereomer, Hz.

	H1'	H2'	H2''	H3'	H4'	H5' & H5''	H5	H6	TpC	Cp*A
H1'	*	8.0	6.0	0	0	0	0	0	0	0
H2'	8.0	*	14.2	6.3	0	0	0	0	0	0
H2''	6.0	14.2	*	2.8	0	0	0	0	0	0
H3'	0	6.3	2.8	*	2.7	0	0	0	0	7.0
H4'	0	0	0	2.7	*	2.8	0	0	n.d..	n.d..
H5' & H5''	0	0	0	0	2.8	11.6	0	0	4.8	0
H5	0	0	0	0	0	0	*	7.6	0	0
H6	0	0	0	0	0	0	7.6	*	0	0
TpC	0	0	0	0	n.d..	4.8	0	0	*	0
Cp*A	0	0	0	7.0	n.d..	0	0	0	0	*

Table 10
Coupling constants $^1\text{H}-^1\text{H}$, $^1\text{H}-^{31}\text{P}$ of cytidine monophosphate of 'slow' diastereomer, Hz.

	H1'	H2'	H2''	H3'	H4'	H5' & H5''	H5	H6	TpC	Cp*A
H1'	*	7.9	6.0	0	0	0	0	0	0	0
H2'	7.9	*	14.2	6.3	0	0	0	0	0	0
H2''	6.0	14.2	*	2.8	0	0	0	0	0	0
H3'	0	6.3	2.8	*	2.8	0	0	0	0	7.0
H4'	0	0	0	2.8	*	3.4	0	0	n.d..	n.d..
H5' & H5''	0	0	0	0	3.4	11.7	0	0	4.2 4.6	0
H5	0	0	0	0	0	0	*	7.5	0	0
H6	0	0	0	0	0	0	7.5	*	0	0
TpC	0	0	0	0	n.d..	4.2, 4.6	0	0	*	0
Cp*A	0	0	0	7.0	n.d..	0	0	0	0	*

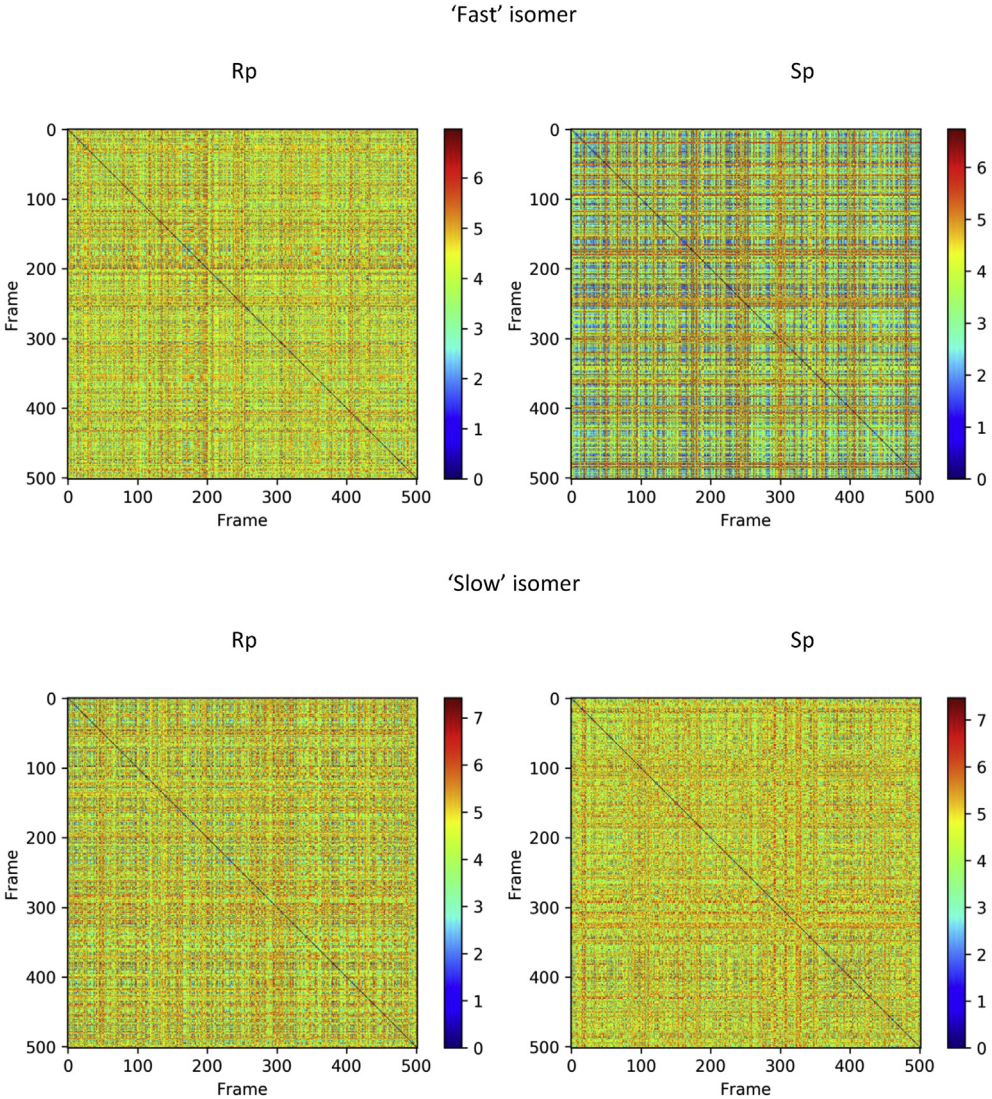


Fig. 10. RMSD map for 500 final structures after simulation annealing. Mixing time 0.4 s.

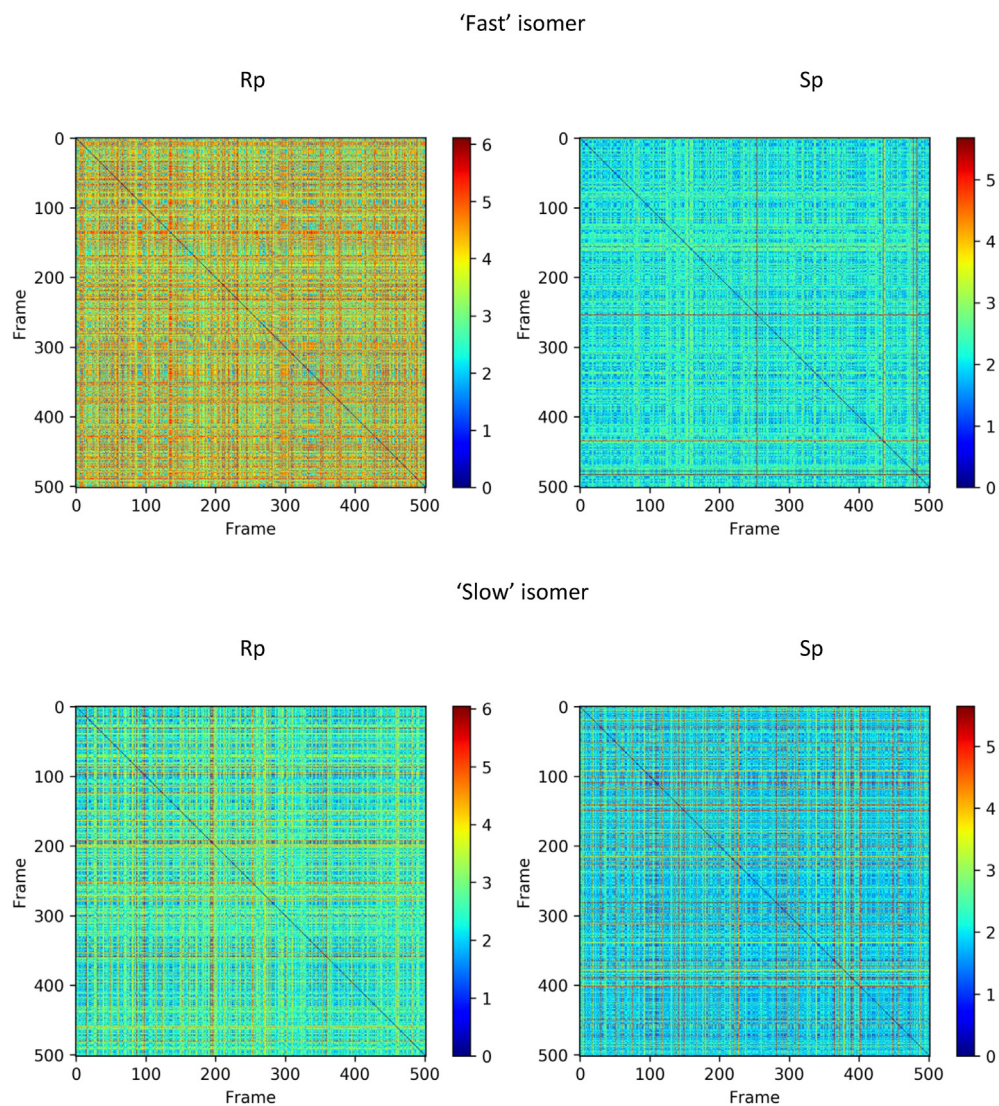


Fig. 11. RMSD map for 500 final structures after simulation annealing. Mixing time 0.8 s.

Table 11

NOESY NMR restraints with mixing time 0.4s of 'fast' trinucleotide and MD restraint penalty values for Rp- and Sp-diastereomers.

#	Residue number, Residue name, Atom Name	Residue number, Residue name, Atom Name	Distance, Å	Restraint penalty, kcal/mol Rp-isomer	Sp-isomer
1	1 dT H1'	1 dT H3'	6.14	0 ± 0	0 ± 0
2	1 dT H1'	1 dT H6	3.12	0.06 ± 0.05	0.08 ± 0.05
3	1 dT H2'2	1 dT H1'	4.03	0 ± 0	0 ± 0
4	1 dT H2'2	1 dT H2'1	2.74	0 ± 0	0 ± 0
5	1 dT H2'2	1 dT H3'	3.57	0 ± 0	0 ± 0
6	1 dT H2'2	1 dT H4'	4.61	0 ± 0	0 ± 0
7	1 dT H2'2	1 dT H6	4.09	0 ± 0.01	0 ± 0.01
8	1 dT H2'1	1 dT H1'	3.52	0 ± 0	0 ± 0
9	1 dT H2'1	1 dT H3'	3.44	0 ± 0	0 ± 0
10	1 dT H2'1	1 dT H6	2.87	0.08 ± 0.13	0.06 ± 0.12
11	1 dT H4'	1 dT H1'	4.10	0 ± 0	0 ± 0
12	1 dT H4'	1 dT H3'	3.46	0 ± 0	0 ± 0
13	1 dT H4'	1 dT H6	4.92	0.03 ± 0.04	0.02 ± 0.04
14	1 dT H5'1	1 dT H3'	3.68	0 ± 0	0 ± 0
15	1 dT H5'1	1 dT H4'	2.67	0.01 ± 0.02	0.01 ± 0.02
16	1 dT H5'1	1 dT H6	4.60	0.18 ± 0.21	0.1 ± 0.17
17	1 dT H5'2	1 dT H3'	3.82	0 ± 0	0 ± 0
18	1 dT H5'2	1 dT H4'	3.32	0 ± 0	0 ± 0
19	1 dT H5'2	1 dT H6	4.84	0.19 ± 0.21	0.11 ± 0.17
20	1 dT H6	1 dT H3'	3.90	0.16 ± 0.17	0.13 ± 0.16
21	1 dT M7	1 dT H6	2.85	0 ± 0	0 ± 0
22	2 dC H1'	2 dC H2'1	3.15	0 ± 0	0 ± 0
23	2 dC H1'	2 dC H5'1	4.49	0.01 ± 0.02	0.01 ± 0.02
24	2 dC H1'	2 dC H5'2	4.61	0.03 ± 0.03	0.02 ± 0.03
25	2 dC H1'	2 dC H6	3.24	0.07 ± 0.02	0.07 ± 0.02
26	2 dC H2'2	2 dC H1'	3.24	0 ± 0	0 ± 0
27	2 dC H2'2	2 dC H2'1	2.71	0 ± 0	0 ± 0
28	2 dC H2'2	2 dC H3'	3.39	0 ± 0	0 ± 0
29	2 dC H2'2	2 dC H5	6.29	0 ± 0	0 ± 0
30	2 dC H2'2	2 dC H6	3.68	0.03 ± 0.04	0.03 ± 0.04
31	2 dC H2'2	2 dC H5'1	5.28	0 ± 0	0 ± 0
32	2 dC H2'2	2 dC H5'2	5.70	0 ± 0	0 ± 0
33	2 dC H2'1	2 dC H5'1	4.45	0.01 ± 0.04	0.02 ± 0.05
34	2 dC H2'1	2 dC H5'2	4.30	0.01 ± 0.04	0.01 ± 0.04
35	2 dC H3'	2 dC H1'	5.76	0 ± 0	0 ± 0
36	2 dC H3'	2 dC H2'1	3.21	0 ± 0	0 ± 0
37	2 dC H3'	2 dC H5'1	3.21	0.04 ± 0.04	0.03 ± 0.04
38	2 dC H3'	2 dC H5'2	3.18	0.02 ± 0.03	0.03 ± 0.04
39	2 dC H3'	2 dC H6	4.17	0.01 ± 0.02	0.01 ± 0.03
40	2 dC H4'	2 dC H5'1	2.31	0.04 ± 0.06	0.07 ± 0.07
41	2 dC H4'	2 dC H5'2	2.43	0.01 ± 0.03	0.01 ± 0.03
42	2 dC H5	2 dC H2'1	4.69	0 ± 0.01	0 ± 0.01
43	2 dC H5	2 dC H5'1	5.84	0.05 ± 0.09	0.06 ± 0.1
44	2 dC H5	2 dC H5'2	6.56	0.04 ± 0.07	0.04 ± 0.07
45	2 dC H5	2 dC H6	2.50	0 ± 0	0 ± 0
46	2 dC H6	2 dC H2'1	2.82	0 ± 0.02	0.01 ± 0.03
47	2 dC H6	2 dC H5'1	3.80	0.04 ± 0.07	0.05 ± 0.08
48	2 dC H6	2 dC H5'2	3.83	0.11 ± 0.11	0.09 ± 0.11
49	3 d(p*A) H1'	3 d(p*A) H8	3.84	0 ± 0	0 ± 0
50	3 d(p*A) H2'2	3 d(p*A) H1'	3.17	0 ± 0	0 ± 0
51	3 d(p*A) H2'2	3 d(p*A) H2'1	2.85	0 ± 0	0 ± 0
52	3 d(p*A) H2'2	3 d(p*A) H3'	3.30	0 ± 0	0 ± 0
53	3 d(p*A) H2'2	3 d(p*A) H8	4.24	0 ± 0.01	0 ± 0
54	3 d(p*A) H2'1	3 d(p*A) H1'	3.21	0 ± 0	0 ± 0
55	3 d(p*A) H2'1	3 d(p*A) H3'	2.94	0 ± 0	0 ± 0
56	3 d(p*A) H2'1	3 d(p*A) H8	3.09	0.01 ± 0.04	0 ± 0.02
57	3 d(p*A) H2	3 d(p*A) H1'	5.20	0 ± 0.02	0 ± 0.02
58	3 d(p*A) H2	3 d(p*A) H2'1	6.46	0.04 ± 0.04	0.05 ± 0.04
59	3 d(p*A) H3'	3 d(p*A) H1'	4.23	0 ± 0	0 ± 0
60	3 d(p*A) H3'	3 d(p*A) H8	3.85	0.13 ± 0.09	0.12 ± 0.08

Table 11 (continued)

#	Residue number, Residue name, Atom Name	Residue number, Residue name, Atom Name	Distance, Å	Restraint penalty, kcal/mol Rp-isomer	Sp-isomer
61	3 d(p*A) H4'	3 d(p*A) H1'	3.59	0 ± 0	0 ± 0
62	3 d(p*A) H4'	3 d(p*A) H2'1	4.36	0 ± 0	0 ± 0
63	3 d(p*A) H4'	3 d(p*A) H2'2	3.88	0.01 ± 0.01	0.01 ± 0.01
64	3 d(p*A) H4'	3 d(p*A) H8	6.02	0 ± 0	0 ± 0
65	1 dT H1'	2 dC H5'1	4.14	0.13 ± 0.22	0.13 ± 0.19
66	1 dT H1'	2 dC H5'2	4.29	0.17 ± 0.22	0.25 ± 0.23
67	1 dT H1'	2 dC H6	5.25	0.07 ± 0.17	0.07 ± 0.15
68	1 dT H2'2	2 dC H6	4.24	0.07 ± 0.19	0.1 ± 0.23
69	1 dT H2'2	2 dC H5'1	4.27	0.03 ± 0.1	0.06 ± 0.14
70	1 dT H2'2	2 dC H5'2	4.45	0.01 ± 0.04	0.02 ± 0.04
71	1 dT H2'1	2 dC H5	5.45	0.18 ± 0.29	0.26 ± 0.29
72	1 dT H2'1	2 dC H6	4.78	0.08 ± 0.18	0.1 ± 0.18
73	1 dT H3'	2 dC H5'1	3.61	0.16 ± 0.16	0.15 ± 0.18
74	1 dT H3'	2 dC H5'2	3.63	0.29 ± 0.18	0.24 ± 0.17
75	1 dT H3'	2 dC H6	4.66	0.1 ± 0.15	0.13 ± 0.15
76	1 dT H6	2 dC H5'1	5.31	0.17 ± 0.24	0.23 ± 0.23
77	1 dT H6	2 dC H5'2	6.06	0.14 ± 0.18	0.23 ± 0.23
78	1 dT M7	2 dC H5	5.86	0.35 ± 0.51	0.46 ± 0.47
79	1 dT H6	3 d(p*A) H2'1	5.83	0.35 ± 0.49	0.29 ± 0.48
80	2 dC H2'2	3 d(p*A) H8	4.85	0.13 ± 0.21	0.09 ± 0.24
81	2 dC H2'1	3 d(p*A) H8	4.95	0.13 ± 0.22	0.09 ± 0.24
82	2 dC H6	3 d(p*A) H2'1	6.73	0.1 ± 0.18	0.09 ± 0.15
83	3 d(p*A) H2	1 dT M7	5.30	0.54 ± 0.52	0.45 ± 0.44
84	3 d(p*A) H8	2 dC H5'1	5.56	0.19 ± 0.29	0.16 ± 0.24
85	3 d(p*A) H8	2 dC H5'2	6.10	0.11 ± 0.19	0.11 ± 0.16
86	1 dT H1'	3 d(p*A) Me	5.53	0.1 ± 0.2	0.05 ± 0.14
87	1 dT H4'	3 d(p*A) Me	4.54	0.58 ± 0.43	0.29 ± 0.42
88	1 dT H6	3 d(p*A) Me	4.98	0.34 ± 0.38	0.17 ± 0.31
89	2 dC H1'	3 d(p*A) Me	4.28	0.08 ± 0.11	0.08 ± 0.1
90	2 dC H3'	3 d(p*A) Me	5.04	0 ± 0	0 ± 0
91	3 d(p*A) H2	3 d(p*A) Me	4.52	0.79 ± 0.64	1.17 ± 0.44
92	3 d(p*A) H4'	3 d(p*A) Me	3.74	0.09 ± 0.12	0.26 ± 0.17
93	3 d(p*A) Me	2 dC H5'1	4.08	0.06 ± 0.1	0.07 ± 0.17
94	3 d(p*A) Me	2 dC H5'2	4.22	0.03 ± 0.08	0.02 ± 0.09
95	3 d(p*A) Me	3 d(p*A) H8	3.72	0.45 ± 0.43	0.17 ± 0.34
96	3 d(p*A) Me	2 dC H6	5.14	0.09 ± 0.1	0.07 ± 0.09
97	1 dT H6	2 dC H4'	6.17	0.17 ± 0.22	0.29 ± 0.23
98	2 dC H1'	2 dC H4'	3.21	0.01 ± 0.02	0.01 ± 0.02
99	2 dC H2'2	2 dC H4'	3.43	0.08 ± 0.05	0.08 ± 0.05
100	2 dC H2'2	3 d(p*A) H5'1	3.43	0.33 ± 0.3	0.13 ± 0.21
101	2 dC H2'2	3 d(p*A) H5'2	3.43	0.2 ± 0.2	0.16 ± 0.16
102	2 dC H2'1	2 dC H4'	4.00	0 ± 0	0 ± 0
103	2 dC H3'	2 dC H4'	3.28	0 ± 0	0 ± 0
104	2 dC H5	2 dC H4'	5.65	0.27 ± 0.06	0.28 ± 0.06
105	2 dC H4'	3 d(p*A) Me	2.92	0.07 ± 0.14	0.1 ± 0.17
106	2 dC H6	2 dC H4'	4.41	0.01 ± 0.03	0.02 ± 0.03
107	3 d(p*A) H1'	3 d(p*A) H5'1	4.37	0.04 ± 0.04	0.02 ± 0.03
108	3 d(p*A) H1'	3 d(p*A) H5'2	4.37	0.04 ± 0.05	0.06 ± 0.04
109	3 d(p*A) H2'2	3 d(p*A) H5'1	4.60	0.06 ± 0.05	0.09 ± 0.05
110	3 d(p*A) H2'2	3 d(p*A) H5'2	4.60	0.02 ± 0.03	0.03 ± 0.03
111	3 d(p*A) H2'1	3 d(p*A) H5'1	3.73	0.06 ± 0.09	0.06 ± 0.07
112	3 d(p*A) H2'1	3 d(p*A) H5'2	3.73	0.03 ± 0.06	0.03 ± 0.06
113	3 d(p*A) H2	3 d(p*A) H5'1	5.48	0.67 ± 0.3	0.62 ± 0.25
114	3 d(p*A) H2	3 d(p*A) H5'2	5.48	0.69 ± 0.23	0.82 ± 0.19
115	3 d(p*A) H3'	3 d(p*A) H5'1	2.98	0.07 ± 0.07	0.11 ± 0.06
116	3 d(p*A) H3'	3 d(p*A) H5'2	2.98	0 ± 0.01	0 ± 0.01
117	3 d(p*A) H8	3 d(p*A) H5'1	4.38	0.16 ± 0.17	0.11 ± 0.15
118	3 d(p*A) H8	3 d(p*A) H5'2	4.38	0.11 ± 0.17	0.18 ± 0.15

Table 12

NOESY NMR restraints with mixing time 0.4s of 'slow' trinucleotide and MD restraint penalty values for Rp- and Sp-diastereomers.

#	Residue number, Residue name, Atom Name	Residue number, Residue name, Atom Name	Distance, Å	Restraint penalty, kcal/mol	
				Rp	Sp
1	1 dT H1'	1 dT H3'	5.84	0 ± 0	0 ± 0
2	1 dT H1'	1 dT H6	2.68	0.23 ± 0.04	0.22 ± 0.06
3	1 dT H2'2	1 dT H1'	3.00	0 ± 0	0 ± 0
4	1 dT H2'2	1 dT H2'1	2.41	0 ± 0	0 ± 0
5	1 dT H2'2	1 dT H3'	3.54	0 ± 0	0 ± 0
6	1 dT H2'2	1 dT H4'	3.82	0.01 ± 0.01	0.01 ± 0.01
7	1 dT H2'2	1 dT H6	3.59	0.06 ± 0.06	0.05 ± 0.06
8	1 dT H2'1	1 dT H3'	2.63	0 ± 0	0 ± 0
9	1 dT H2'1	1 dT H6	2.36	0.06 ± 0.09	0.07 ± 0.12
10	1 dT H4'	1 dT H1'	3.55	0 ± 0	0 ± 0
11	1 dT H4'	1 dT H3'	2.81	0 ± 0	0 ± 0
12	1 dT H4'	1 dT H6	3.98	0.09 ± 0.06	0.1 ± 0.08
13	1 dT H5'1	1 dT H3'	2.90	0.11 ± 0.07	0.11 ± 0.07
14	1 dT H5'1	1 dT H4'	4.45	0 ± 0	0 ± 0
15	1 dT H5'1	1 dT H6	3.64	0.08 ± 0.13	0.12 ± 0.18
16	1 dT H5'2	1 dT H3'	2.85	0.03 ± 0.06	0.03 ± 0.07
17	1 dT H5'2	1 dT H4'	2.27	0.03 ± 0.05	0.03 ± 0.05
18	1 dT H5'2	1 dT H6	3.54	0.25 ± 0.18	0.26 ± 0.21
19	1 dT H6	1 dT H3'	3.24	0.28 ± 0.11	0.28 ± 0.11
20	1 dT M7	1 dT H6	2.41	0 ± 0	0 ± 0
21	2 dC H1'	2 dC H2'1	2.88	0.01 ± 0.01	0.01 ± 0.01
22	2 dC H1'	2 dC H4'	2.83	0.04 ± 0.04	0.04 ± 0.04
23	2 dC H1'	2 dC H6	2.79	0.2 ± 0.03	0.2 ± 0.02
24	2 dC H2'2	2 dC H1'	2.42	0 ± 0	0 ± 0
25	2 dC H2'2	2 dC H2'1	2.14	0 ± 0	0 ± 0
26	2 dC H2'2	2 dC H3'	3.28	0 ± 0	0 ± 0
27	2 dC H2'2	2 dC H4'	2.97	0.22 ± 0.06	0.21 ± 0.06
28	2 dC H2'2	2 dC H6	3.09	0.17 ± 0.08	0.17 ± 0.07
29	2 dC H2'1	2 dC H4'	3.47	0.05 ± 0.03	0.04 ± 0.02
30	2 dC H3'	2 dC H2'1	2.89	0 ± 0	0 ± 0
31	2 dC H3'	2 dC H6	3.89	0.06 ± 0.07	0.05 ± 0.05
32	2 dC H5	2 dC H6	2.50	0 ± 0	0 ± 0
33	2 dC H6	2 dC H2'1	2.44	0.03 ± 0.06	0.02 ± 0.05
34	2 dC H6	2 dC H4'	3.77	0.16 ± 0.07	0.13 ± 0.06
35	3 d(p'A) H1'	3 d(p'A) H5'2	3.12	0.37 ± 0.1	0.38 ± 0.1
36	3 d(p'A) H1'	3 d(p'A) H8	3.26	0.09 ± 0.04	0.09 ± 0.04
37	3 d(p'A) H2'2	3 d(p'A) H1'	2.48	0 ± 0	0 ± 0
38	3 d(p'A) H2'2	3 d(p'A) H2'1	2.35	0 ± 0	0 ± 0
39	3 d(p'A) H2'2	3 d(p'A) H3'	3.45	0 ± 0	0 ± 0
40	3 d(p'A) H2'2	3 d(p'A) H5'1	3.71	0.3 ± 0.08	0.3 ± 0.1
41	3 d(p'A) H2'2	3 d(p'A) H8	3.76	0.02 ± 0.05	0.02 ± 0.04
42	3 d(p'A) H2'1	3 d(p'A) H1'	3.20	0 ± 0	0 ± 0
43	3 d(p'A) H2'1	3 d(p'A) H3'	2.67	0 ± 0	0 ± 0
44	3 d(p'A) H2'1	3 d(p'A) H5'1	3.19	0.18 ± 0.12	0.19 ± 0.13
45	3 d(p'A) H2'1	3 d(p'A) H5'2	3.17	0.09 ± 0.12	0.12 ± 0.13
46	3 d(p'A) H2'1	3 d(p'A) H8	2.53	0.03 ± 0.1	0.02 ± 0.05
47	3 d(p'A) H3'	3 d(p'A) H1'	4.00	0 ± 0	0 ± 0
48	3 d(p'A) H3'	3 d(p'A) H5'1	2.57	0.12 ± 0.13	0.14 ± 0.13
49	3 d(p'A) H3'	3 d(p'A) H5'2	2.45	0.03 ± 0.04	0.04 ± 0.06
50	3 d(p'A) H3'	3 d(p'A) H8	3.32	0.27 ± 0.13	0.25 ± 0.1
51	3 d(p'A) H4'	3 d(p'A) H1'	3.02	0.02 ± 0.03	0.02 ± 0.04
52	3 d(p'A) H4'	3 d(p'A) H2'1	3.16	0.12 ± 0.03	0.13 ± 0.03
53	3 d(p'A) H4'	3 d(p'A) H2'2	3.18	0.16 ± 0.06	0.16 ± 0.06
54	3 d(p'A) H8	3 d(p'A) H5'1	3.79	0.3 ± 0.25	0.25 ± 0.2
55	3 d(p'A) H8	3 d(p'A) H5'2	3.84	0.18 ± 0.19	0.19 ± 0.2
56	1 dT H3'	2 dC H6	3.81	0.47 ± 0.28	0.53 ± 0.27
57	2 dC H2'2	3 d(p'A) H5'2	3.76	0.17 ± 0.16	0.22 ± 0.21
58	2 dC H2'1	3 d(p'A) H8	4.13	0.65 ± 0.46	0.54 ± 0.44

Table 12 (continued)

#	Residue number, Residue name, Atom Name	Residue number, Residue name, Atom Name	Distance, Å	Restraint penalty, kcal/mol	
				Rp	Sp
59	3 d(p*A) H8	2 dC H4'	3.69	0.5 ± 0.49	0.54 ± 0.47
60	1 dT H1'	2 dC H5'1	3.39	0.31 ± 0.32	0.35 ± 0.22
61	1 dT H1'	2 dC H5'2	3.39	0.18 ± 0.16	0.17 ± 0.26
62	2 dC H2'2	2 dC H5'1	3.12	0.52 ± 0.51	0.51 ± 0.11
63	2 dC H2'2	2 dC H5'2	3.12	0.42 ± 0.42	0.44 ± 0.08
64	2 dC H2'1	2 dC H5'1	3.26	0.22 ± 0.2	0.21 ± 0.12
65	2 dC H2'1	2 dC H5'2	3.26	0.14 ± 0.14	0.16 ± 0.1
66	2 dC H3'	2 dC H5'1	2.83	0.14 ± 0.13	0.13 ± 0.07
67	2 dC H3'	2 dC H5'2	2.83	0.01 ± 0.01	0.02 ± 0.06
68	2 dC H4'	2 dC H5'1	1.89	0.1 ± 0.1	0.1 ± 0.06
69	2 dC H4'	2 dC H5'2	1.89	0.11 ± 0.11	0.1 ± 0.06
70	2 dC H6	2 dC H5'1	3.17	0.2 ± 0.18	0.16 ± 0.14
71	2 dC H6	2 dC H5'2	3.17	0.3 ± 0.3	0.3 ± 0.16
72	1 dT H1'	3 d(p*A) Me	4.25	0.19 ± 0.15	0.2 ± 0.38
73	1 dT H4'	3 d(p*A) Me	3.68	0.4 ± 0.39	0.38 ± 0.53
74	2 dC H1'	3 d(p*A) Me	3.55	0.22 ± 0.23	0.2 ± 0.19
75	2 dC H4'	3 d(p*A) Me	2.80	0.18 ± 0.17	0.23 ± 0.25
76	2 dC H6	3 d(p*A) Me	4.22	0.34 ± 0.38	0.44 ± 0.14
77	3 d(p*A) Me	2 dC H5'1	3.09	0.4 ± 0.39	0.49 ± 0.4
78	3 d(p*A) Me	2 dC H5'2	3.09	0.23 ± 0.23	0.32 ± 0.33
79	3 d(p*A) H2	3 d(p*A) Me	3.90	0.85 ± 0.88	1.19 ± 0.62
80	3 d(p*A) H3'	2 dC H5'1	3.10	0.95 ± 0.98	1.14 ± 0.52
81	3 d(p*A) H3'	2 dC H5'2	3.10	0.84 ± 0.87	0.98 ± 0.48

Table 13

NOESY NMR restraints with mixing time 0.8s of 'fast' trinucleotide and MD restraint penalty values for Rp- and Sp-diastereomers.

#	Residue number, Residue name, Atom Name	Residue number, Residue name, Atom Name	Distance, Å	Restraint penalty, kcal/mol	
				Rp	Sp
1	1 dT H1'	1 dT H3'	4.65	0 ± 0	0 ± 0
2	1 dT H1'	1 dT H6	2.80	0.59 ± 0.61	8.13 ± 1.68
3	1 dT H2'2	1 dT H1'	3.46	0 ± 0	0 ± 0.01
4	1 dT H2'2	1 dT H2'1	2.68	0.1 ± 0.14	0.06 ± 0.1
5	1 dT H2'2	1 dT H3'	3.55	0 ± 0	0 ± 0
6	1 dT H2'2	1 dT H4'	4.35	0 ± 0	0 ± 0
7	1 dT H2'2	1 dT H6	3.59	0 ± 0	0.02 ± 0.09
8	1 dT H2'1	1 dT H1'	4.12	0 ± 0	0 ± 0
9	1 dT H2'1	1 dT H3'	3.05	0 ± 0	0 ± 0
10	1 dT H2'1	1 dT H6	2.66	0 ± 0	0 ± 0
11	1 dT H4'	1 dT H1'	3.65	0.04 ± 0.12	0.17 ± 0.31
12	1 dT H4'	1 dT H3'	3.19	0 ± 0	0 ± 0
13	1 dT H4'	1 dT H6	4.49	7.82 ± 1.58	0.1 ± 0.21
14	1 dT H5'1	1 dT H3'	3.33	0 ± 0	0.19 ± 0.49
15	1 dT H5'1	1 dT H4'	2.82	0.11 ± 0.21	0.32 ± 0.42
16	1 dT H5'1	1 dT H6	4.09	0.51 ± 0.69	0.02 ± 0.11
17	1 dT H5'2	1 dT H3'	3.42	0.19 ± 0.31	0.38 ± 0.58
18	1 dT H5'2	1 dT H4'	2.78	0.32 ± 0.34	0.22 ± 0.44
19	1 dT H5'2	1 dT H6	3.96	0.33 ± 0.61	0.1 ± 0.33
20	1 dT H6	1 dT H3'	3.44	6.01 ± 1.81	0.31 ± 0.5
21	1 dT M7	1 dT H6	2.59	0 ± 0	0 ± 0
22	2 dC H1'	2 dC H2'1	3.19	0 ± 0	0 ± 0
23	2 dC H1'	2 dC H5'1	3.99	0.05 ± 0.13	1.03 ± 0.62
24	2 dC H1'	2 dC H5'2	4.07	1.42 ± 0.89	0 ± 0
25	2 dC H1'	2 dC H6	2.86	5.02 ± 1.23	1.86 ± 1.05
26	2 dC H2'2	2 dC H1'	2.72	0 ± 0	0 ± 0

(continued on next page)

Table 13 (continued)

#	Residue number, Residue name, Atom Name	Residue number, Residue name, Atom Name	Distance, Å	Restraint penalty, kcal/mol	
				Rp	Sp
27	2 dC H2'2	2 dC H2'1	2.51	0.12 ± 0.15	0.19 ± 0.2
28	2 dC H2'2	2 dC H3'	3.24	0 ± 0	0 ± 0
29	2 dC H2'2	2 dC H5	4.48	2.34 ± 1.38	2.75 ± 1.52
30	2 dC H2'2	2 dC H6	3.24	2.37 ± 1.1	0 ± 0
31	2 dC H2'2	2 dC H5'1	4.64	0 ± 0	0 ± 0
32	2 dC H2'2	2 dC H5'2	4.81	0.04 ± 0.13	0 ± 0
33	2 dC H2'1	2 dC H5'1	4.04	0 ± 0	0 ± 0
34	2 dC H2'1	2 dC H5'2	3.93	0 ± 0	0 ± 0
35	2 dC H3'	2 dC H1'	4.65	0 ± 0	0 ± 0
36	2 dC H3'	2 dC H2'1	2.98	0 ± 0	0 ± 0
37	2 dC H3'	2 dC H5'1	2.93	0 ± 0.01	0 ± 0
38	2 dC H3'	2 dC H5'2	2.91	4.07 ± 1.28	1.54 ± 0.85
39	2 dC H3'	2 dC H6	3.89	0.7 ± 0.63	0.44 ± 0.45
40	2 dC H4'	2 dC H5'1	2.14	9.65 ± 1.32	5.31 ± 1.5
41	2 dC H4'	2 dC H5'2	2.14	0.05 ± 0.13	7.65 ± 1.49
42	2 dC H5	2 dC H2'1	4.01	0 ± 0	0.04 ± 0.09
43	2 dC H5	2 dC H5'1	4.81	0 ± 0	0.54 ± 0.59
44	2 dC H5	2 dC H5'2	4.84	1.31 ± 1.1	0 ± 0
45	2 dC H5	2 dC H6	2.50	0 ± 0.01	0 ± 0
46	2 dC H6	2 dC H2'1	2.63	0 ± 0.01	0 ± 0.01
47	2 dC H6	2 dC H5'1	3.43	0 ± 0	0.17 ± 0.26
48	2 dC H6	2 dC H5'2	3.42	0 ± 0	0.01 ± 0.05
49	3 d(p'A) H1'	3 d(p'A) H8	3.41	2.03 ± 0.77	1.35 ± 0.66
50	3 d(p'A) H2'2	3 d(p'A) H1'	2.64	0 ± 0	0 ± 0
51	3 d(p'A) H2'2	3 d(p'A) H2'1	2.83	0.04 ± 0.08	0.06 ± 0.12
52	3 d(p'A) H2'2	3 d(p'A) H3'	3.60	0 ± 0	0 ± 0
53	3 d(p'A) H2'2	3 d(p'A) H8	3.92	0.58 ± 0.49	1.14 ± 0.72
54	3 d(p'A) H2'1	3 d(p'A) H1'	3.38	0 ± 0	0 ± 0
55	3 d(p'A) H2'1	3 d(p'A) H3'	3.14	0 ± 0	0 ± 0
56	3 d(p'A) H2'1	3 d(p'A) H8	2.82	0.23 ± 0.38	0.09 ± 0.21
57	3 d(p'A) H2	3 d(p'A) H1'	4.06	0.41 ± 0.49	1.9 ± 1.08
58	3 d(p'A) H2	3 d(p'A) H2'1	4.47	5.3 ± 2.65	0.73 ± 0.78
59	3 d(p'A) H3'	3 d(p'A) H1'	3.97	0.02 ± 0.07	0.02 ± 0.07
60	3 d(p'A) H3'	3 d(p'A) H8	3.46	0 ± 0	1.34 ± 1.11
61	3 d(p'A) H4'	3 d(p'A) H1'	3.15	0.4 ± 0.46	0.13 ± 0.26
62	3 d(p'A) H4'	3 d(p'A) H2'1	3.59	1.53 ± 0.75	1.24 ± 0.71
63	3 d(p'A) H4'	3 d(p'A) H2'2	3.50	0 ± 0	0.34 ± 0.47
64	3 d(p'A) H4'	3 d(p'A) H8	4.22	0 ± 0.03	0.07 ± 0.16
65	1 dT H1'	2 dC H5'1	3.70	0.79 ± 0.81	3.59 ± 1.59
66	1 dT H1'	2 dC H5'2	3.72	0 ± 0	0.84 ± 0.69
67	1 dT H1'	2 dC H6	4.36	0.11 ± 0.22	0.16 ± 0.33
68	1 dT H2'2	2 dC H6	3.94	0 ± 0	0 ± 0
69	1 dT H2'2	2 dC H5'1	3.97	0 ± 0	0 ± 0
70	1 dT H2'2	2 dC H5'2	4.09	0 ± 0	0 ± 0
71	1 dT H2'1	2 dC H5	4.54	0 ± 0.03	0 ± 0
72	1 dT H2'1	2 dC H6	3.78	0.02 ± 0.09	0 ± 0
73	1 dT H3'	2 dC H5'1	3.35	0.11 ± 0.21	0 ± 0
74	1 dT H3'	2 dC H5'2	3.34	0.44 ± 0.49	0.44 ± 0.5
75	1 dT H3'	2 dC H6	4.08	0.34 ± 0.46	1.2 ± 0.88
76	1 dT H6	2 dC H5'1	4.52	0 ± 0.02	0 ± 0.03
77	1 dT H6	2 dC H5'2	4.65	0 ± 0	0.73 ± 0.82
78	1 dT M7	2 dC H5	4.46	0.05 ± 0.19	0 ± 0.03
79	1 dT H6	3 d(p'A) H2'1	5.38	0.01 ± 0.13	0.35 ± 0.57
80	2 dC H2'2	3 d(p'A) H8	4.28	2.01 ± 1.31	0 ± 0
81	2 dC H2'1	3 d(p'A) H8	4.35	1.44 ± 0.78	0 ± 0
82	2 dC H6	3 d(p'A) H2'1	4.72	1.38 ± 1.11	0.14 ± 0.35
83	3 d(p'A) H2	1 dT M7	4.87	0.29 ± 0.49	0 ± 0
84	3 d(p'A) H8	2 dC H5'1	5.93	0 ± 0	0 ± 0
85	3 d(p'A) H8	2 dC H5'2	5.41	0 ± 0	0.97 ± 0.83
86	1 dT H1'	3 d(p'A) Me	4.92	0 ± 0	0 ± 0

Table 13 (continued)

#	Residue number, Residue name, Atom Name	Residue number, Residue name, Atom Name	Distance, Å	Restraint penalty, kcal/mol	
				Rp	Sp
87	1 dT H4'	3 d(p*A) Me	4.32	0.79 ± 0.82	0.17 ± 0.39
88	1 dT H6	3 d(p*A) Me	4.84	0.21 ± 0.39	0 ± 0
89	2 dC H1'	3 d(p*A) Me	4.02	0.05 ± 0.16	0.04 ± 0.17
90	2 dC H3'	3 d(p*A) Me	3.86	0 ± 0	0 ± 0
91	3 d(p*A) H2	3 d(p*A) Me	4.07	1.46 ± 1.17	0.87 ± 0.95
92	3 d(p*A) H4'	3 d(p*A) Me	3.42	0.18 ± 0.43	0.45 ± 0.56
93	3 d(p*A) Me	2 dC H5'1	3.71	0 ± 0.03	0 ± 0
94	3 d(p*A) Me	2 dC H5'2	3.82	0 ± 0	0.34 ± 0.51
95	3 d(p*A) Me	3 d(p*A) H8	3.02	0 ± 0.03	0.24 ± 0.46
96	3 d(p*A) Me	2 dC H6	4.64	0.03 ± 0.11	0 ± 0

Table 14

NOESY NMR restraints with mixing time 0.8s of 'slow' trinucleotide and MD restraint penalty values for Rp- and Sp-diastereomers.

#	Residue number, Residue name, Atom Name	Residue number, Residue name, Atom Name	Distance, Å	Restraint penalty, kcal/mol	
				Rp	Sp
1	1 dT H1'	1 dT H3'	4.65	0 ± 0	0 ± 0
2	1 dT H1'	1 dT H3'	4.32	0 ± 0	0 ± 0
3	1 dT H1'	1 dT H6	2.74	9.62 ± 1.93	9.52 ± 1.92
4	1 dT H2'2	1 dT H1'	3.35	0 ± 0	0 ± 0
5	1 dT H2'2	1 dT H2'1	2.90	0.07 ± 0.11	0.07 ± 0.1
6	1 dT H2'2	1 dT H3'	3.43	0 ± 0	0 ± 0
7	1 dT H2'2	1 dT H4'	4.12	0 ± 0.03	0 ± 0.01
8	1 dT H2'2	1 dT H6	3.54	0.3 ± 0.48	0.34 ± 0.52
9	1 dT H2'1	1 dT H3'	2.98	0 ± 0	0 ± 0
10	1 dT H2'1	1 dT H6	2.58	0 ± 0.01	0 ± 0.03
11	1 dT H4'	1 dT H1'	3.59	0.15 ± 0.41	0.13 ± 0.37
12	1 dT H4'	1 dT H3'	3.21	0 ± 0	0 ± 0
13	1 dT H4'	1 dT H6	4.36	0.06 ± 0.21	0.07 ± 0.24
14	1 dT H5'1	1 dT H3'	3.38	0.19 ± 0.42	0.16 ± 0.37
15	1 dT H5'1	1 dT H4'	3.12	0 ± 0.01	0 ± 0.02
16	1 dT H5'1	1 dT H6	4.03	0.07 ± 0.3	0.08 ± 0.28
17	1 dT H5'2	1 dT H3'	3.46	0.12 ± 0.26	0.12 ± 0.28
18	1 dT H5'2	1 dT H4'	2.78	0.29 ± 0.56	0.25 ± 0.45
19	1 dT H5'2	1 dT H6	3.80	0.21 ± 0.44	0.23 ± 0.52
20	1 dT H6	1 dT H3'	3.35	0.32 ± 0.63	0.3 ± 0.55
21	1 dT M7	1 dT H6	2.48	0.01 ± 0.04	0.01 ± 0.04
22	2 dC H1'	2 dC H2'1	3.16	0 ± 0	0 ± 0
23	2 dC H1'	2 dC H4'	2.98	0.19 ± 0.37	0.28 ± 0.47
24	2 dC H1'	2 dC H6	2.93	5.3 ± 1.28	5.22 ± 1.32
25	2 dC H2'2	2 dC H1'	2.64	0 ± 0	0 ± 0
26	2 dC H2'2	2 dC H2'1	2.49	0.12 ± 0.15	0.13 ± 0.16
27	2 dC H2'2	2 dC H3'	3.56	0 ± 0	0 ± 0
28	2 dC H2'2	2 dC H4'	3.30	0.01 ± 0.05	0 ± 0.02
29	2 dC H2'2	2 dC H6	3.18	2.58 ± 1.25	2.57 ± 1.25
30	2 dC H2'1	2 dC H4'	3.70	0.16 ± 0.24	0.17 ± 0.26
31	2 dC H3'	2 dC H2'1	3.33	0 ± 0	0 ± 0
32	2 dC H3'	2 dC H6	4.27	0 ± 0	0 ± 0
33	2 dC H5	2 dC H6	2.50	0.1 ± 0.17	0.1 ± 0.16
34	2 dC H6	2 dC H2'1	2.70	0 ± 0.02	0 ± 0.03
35	2 dC H6	2 dC H4'	3.99	0.55 ± 0.68	0.55 ± 0.67
36	3 d(p*A) H1'	3 d(p*A) H5'2	3.91	0.93 ± 0.7	0.98 ± 0.74
37	3 d(p*A) H1'	3 d(p*A) H8	3.27	3.46 ± 1.12	3.53 ± 1.22
38	3 d(p*A) H2'2	3 d(p*A) H1'	2.63	0 ± 0	0 ± 0

(continued on next page)

Table 14 (continued)

#	Residue number, Residue name, Atom Name	Residue number, Residue name, Atom Name	Distance, Å	Restraint penalty, kcal/mol	
				Rp	Sp
39	3 d(p*A) H2'2	3 d(p*A) H2'1	2.82	0.03 ± 0.06	0.03 ± 0.07
40	3 d(p*A) H2'2	3 d(p*A) H3'	3.51	0 ± 0	0 ± 0
41	3 d(p*A) H2'2	3 d(p*A) H5'1	6.02	0 ± 0	0 ± 0
42	3 d(p*A) H2'2	3 d(p*A) H8	3.81	0.09 ± 0.23	0.07 ± 0.18
43	3 d(p*A) H2'1	3 d(p*A) H1'	3.27	0 ± 0	0 ± 0
44	3 d(p*A) H2'1	3 d(p*A) H3'	2.94	0 ± 0	0 ± 0
45	3 d(p*A) H2'1	3 d(p*A) H5'1	3.57	0.46 ± 0.61	0.42 ± 0.63
46	3 d(p*A) H2'1	3 d(p*A) H5'2	3.46	0 ± 0.01	0 ± 0
47	3 d(p*A) H2'1	3 d(p*A) H8	2.73	0 ± 0	0 ± 0.02
48	3 d(p*A) H3'	3 d(p*A) H1'	3.91	0.04 ± 0.11	0.03 ± 0.09
49	3 d(p*A) H3'	3 d(p*A) H5'1	3.01	0 ± 0	0 ± 0
50	3 d(p*A) H3'	3 d(p*A) H5'2	3.09	0 ± 0.01	0 ± 0.01
51	3 d(p*A) H3'	3 d(p*A) H8	3.35	1.18 ± 1.12	1.37 ± 1.17
52	3 d(p*A) H4'	3 d(p*A) H1'	3.09	0.27 ± 0.46	0.17 ± 0.33
53	3 d(p*A) H4'	3 d(p*A) H2'1	3.36	2.67 ± 0.98	2.68 ± 1.06
54	3 d(p*A) H4'	3 d(p*A) H2'2	3.47	1.26 ± 0.88	1.3 ± 0.83
55	3 d(p*A) H8	3 d(p*A) H5'1	4.10	0.03 ± 0.13	0.03 ± 0.13
56	3 d(p*A) H8	3 d(p*A) H5'2	4.33	0 ± 0	0 ± 0
57	1 dT H3'	2 dC H6	4.02	0.04 ± 0.21	0.04 ± 0.18
58	2 dC H2'2	3 d(p*A) H5'2	4.35	0 ± 0	0 ± 0
59	2 dC H2'1	3 d(p*A) H8	4.52	0.32 ± 0.62	0.5 ± 0.7
60	3 d(p*A) H8	2 dC H4'	4.09	0.03 ± 0.16	0 ± 0.02

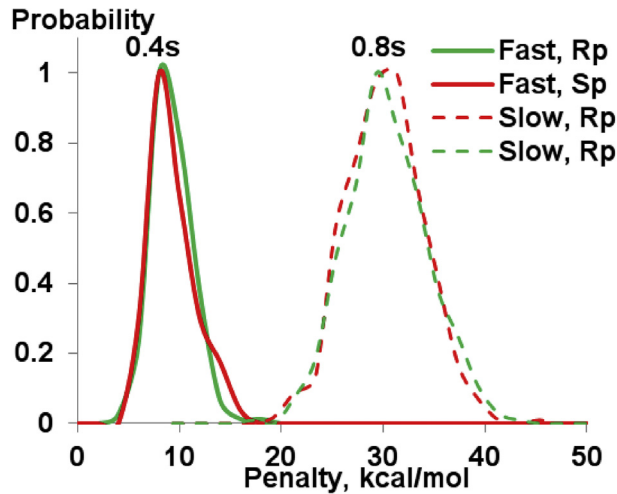


Fig. 12. Distribution of total NMR distance energy penalties obtained in molecular dynamics simulation annealing analysis using distance restraints obtained from NOESY NMR data for 'fast' and 'slow' diastereomers applied for Rp- and Sp-substituted trinucleotides with mixing times 0.4 and 0.8 s. The distributions with the different penalties for the diastereomers are shown in Fig. 4 in Ref. [1].

Table 15

Total restraint penalty energies (in kcal/mol) calculated for the last frame of MD simulation annealing.

Mixing time	'fast' TpCp*A		'slow' TpCp*A	
	Rp	Sp	Rp	Sp
0.4s	10.52 ± 2.02	10.45 ± 2.28	13.35 ± 1.48	14.30 ± 1.43
0.8s	25.47 ± 3.54	23.71 ± 2.86	31.20 ± 3.85	31.45 ± 4.10

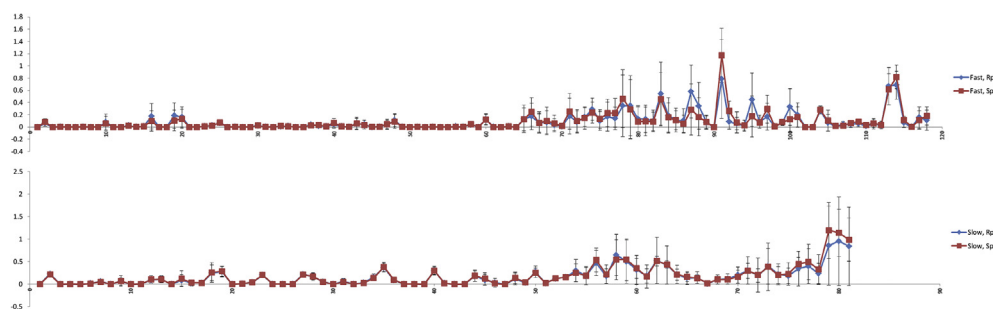


Fig. 13. Comparison of average restraint penalty energy values (in *kcal/mol*) calculated for final structures of 500 annealing simulations for the 'fast' and 'slow' isomers (NOESY NMR mixing time 0.4 s). The number in horizontal axis corresponds to the serial number of restraint in Tables S11–S12. Bars are standard deviations.

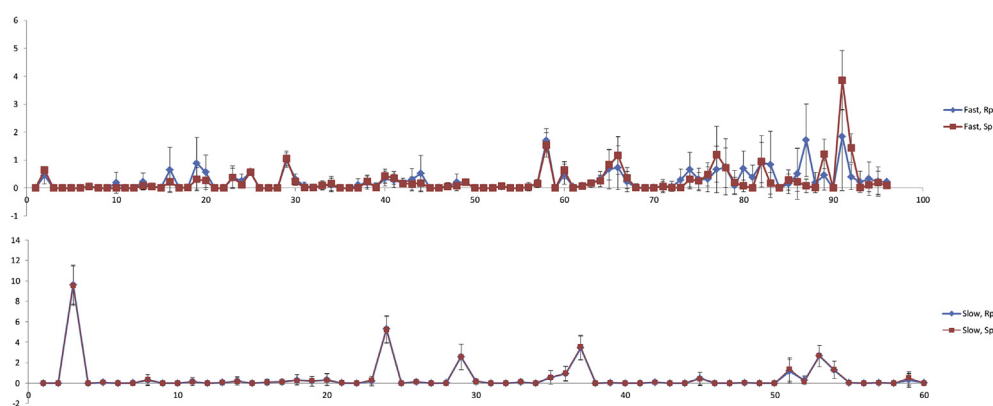


Fig. 14. Comparison of average restraint penalty energy values (in *kcal/mol*) calculated for final structures of 500 annealing simulations for the 'fast' and 'slow' isomers (NOESY NMR mixing time 0.8 s). The number in horizontal axis corresponds to the serial number of restraint in Tables S11–S12. Bars are standard deviations.

Table 16

Summary of the cluster analysis of Rp-isomer using NOESY NMR restraints of 'slow' trinucleotide with mixing time 0.4s.

#Cluster	Frames	Frac	AvgDist	Stdev	AvgCDist
0	12508	0.489	3.487	0.961	5.056
1	5193	0.203	3.169	0.808	4.95
2	3829	0.15	3.673	0.823	5.041
3	1114	0.044	3.189	0.777	5.083
4	1030	0.04	3.595	0.78	5.082
5	937	0.037	3.55	0.764	4.962
6	651	0.025	3.253	0.795	5.178
7	204	0.008	3.506	0.834	5.031
8	113	0.004	3.41	0.817	4.972
9	23	0.001	2.392	0.617	5.171

Abbreviations [4].

#Cluster - Cluster number starting from 0 (0 is most populated).

Frames - number of frames in cluster.

Frac - Size of cluster as fraction of total trajectory.

AvgDist - Average distance between points in the cluster.

Stdev - Standard deviation of points in the cluster.

AvgCDist - Average distance of this cluster to every other cluster.

Table 17

Summary of the cluster analysis of Sp-isomer using NOESY NMR restraints of 'fast' trinucleotide with mixing time 0.4s.

#Cluster	Frames	Frac	AvgDist	Stdev	AvgCDist
0	15544	0.607	2.485	0.706	5.075
1	4380	0.171	2.705	0.619	4.839
2	2390	0.093	3.155	0.783	4.924
3	1531	0.06	3.209	0.764	4.974
4	854	0.033	2.964	0.697	5.165
5	801	0.031	3.018	0.755	5.035
6	67	0.003	2.695	0.663	4.684
7	23	0.001	2.237	0.689	4.846
8	9	0	2.341	0.583	4.728
9	3	0	1.422	0.172	5.073

Table 18

Summary of the cluster analysis of Rp-isomer using NOESY NMR restraints of 'slow' trinucleotide with mixing time 0.8s.

#Cluster	Frames	Frac	AvgDist	Stdev	AvgCDist
0	12193	0.476	2.434	0.482	3.536
1	10952	0.428	2.003	0.466	4.101
2	1005	0.039	2.305	0.523	3.889
3	697	0.027	2.606	0.515	3.51
4	469	0.018	2.167	0.511	3.899
5	231	0.009	2.381	0.441	3.925
6	31	0.001	2.091	0.495	3.483
7	18	0.001	2.113	0.437	3.653
8	4	0	1.41	0.237	4.188
9	2	0	1.798	0	3.967

Table 19

Summary of the cluster analysis of Sp-isomer using NOESY NMR restraints of 'fast' trinucleotide with mixing time 0.8s.

#Cluster	Frames	Frac	AvgDist	Stdev	AvgCDist
0	25264	0.987	2.337	0.474	3.895
1	150	0.006	2.4	0.508	4.439
2	102	0.004	1.993	0.498	3.958
3	50	0.002	1.603	0.398	4.764
4	14	0.001	2.165	0.617	4.185
5	6	0	2.232	0.357	3.935
6	5	0	2.236	0.52	4.481
7	5	0	2.175	0.639	4.084
8	3	0	2.055	0.428	4.231
9	3	0	2.203	0.459	4.247

Acknowledgements

The work was supported by the Russian Science Foundation [grant No. 18-14-00357]. M.S.K. thanks RFBR for financial support [grants No. 16-04-01029] for oligonucleotide synthesis and separation. I.S.D. would like to acknowledge financial support by Russian State funded budget project [0309-2016-0004]. The authors are grateful to the Multi-Access Chemical Research Center of SB RAS for spectral and analytical measurements.

Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.dib.2019.104148>.

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