

NANO IDEA

Open Access



Can Nucleobase Pairs Offer a Possibility of a Direct 3D Self-assembly?

Andrey N. Glushenkov*  and Dmytro M. Hovorun

Abstract

Background: The nucleobase pairs are characterized by their conformational diversity in the wild. Yet a modern nanobiotechnology utilizes their planar conformations only, developing what can be called a “planar approach”. It is well established that the most energetically favorable conformations of the complementary nucleobase pairs are planar and correspond to the classical Watson-Crick nucleobase pairs.

Presentation of the Hypothesis: The point of interest lies in a study of a conformational capacity of the nucleobase pairs to expand the diversity of a spatial configuration and to produce the complex 3D objects from the non-planar conformations. If such a goal could be achieved, then that could definitely open the perspectives for a novel “stereo approach”.

Testing the Hypothesis: For the first time, basing on the first principles, we reveal an ability of the heteroassociates of the $m^1\text{Cyt} \cdot m^1\text{Thy}$ to form up to ten observable molecular complexes under standard conditions. The first three of them have population of ~90 % at standard conditions and are highly non-planar. The most energetically favorable structure has a T-shape, while the next two have an L-shape. At the same time, we show the lack of any experimental data covering a self-assembly of the $m^1\text{Cyt} \cdot m^1\text{Thy}$ base pairs.

Implications of the Hypothesis: We present a theoretical evidence of the fact that the conformational capacity of the nucleobase pairs is much richer from the perspective of their self-assembly than it is considered in the modern nanobiotechnology. The capability of a modified cytosine and a modified thymine to create significantly non-planar structures opens a way for the innovative “stereo approach” to construction of the nanobiotechnological devices. We believe that a modern nanobiotechnological basis can and should be extended with the new nucleic base pairs with innate ability for non-planar structures. We would like to especially emphasize a prognostic role of our algorithm in obtaining the new results.

Keywords: Nucleobase pairs, Non-canonical base pairs, Non-planar base pairs, Nanobiotechnology, Cytosine-thymine, DFT, AIM, NBO, Self-assembly, 3D self-assembly

Background

The modern nanobiotechnology uses the planar building elements for construction of the sophisticated synthetic DNA and RNA [1, 2]. Such elements are complementary base pairs of the adenine-thymine and the guanine-cytosine. This kind of approach allows the creation of a complex spatial structure from the separate modules called “tiles” [3–5]. The resulting structure is a bulk because of the need to bypass an immanent planarity of the complementary nucleobase pairs. In general, this

approach originates in the historically acquired planar X-ray structures [6, 7], may be called “planar”. As one can see, this planar approach was determinative for choosing the base pairs self-assembly types that have been observed experimentally [8].

At the same time, the RNA shows a bigger diversity in the types of interacting base pairs [9] and employs both the canonical and non-canonical base pairs, which results in a rich variety of the secondary and tertiary structures of the RNA. It is obvious that the RNA crystal is capable of creating the non-canonical interactions as well as the non-planar forms of the nucleobase pairs by means of restriction of the degrees of freedom. This fact

* Correspondence: an.glushenkov@yandex.ru

Department of Molecular and Quantum Biophysics, Institute of Molecular Biology and Genetics, NAS of Ukraine, Zabolotnogo Str., 150, Kyiv 03680, Ukraine

allows us to raise a question of the conformational capacity of the electron structures of the different nucleobase pairs. Does the free self-assembly of the essentially planar nucleic bases result in strictly planar base pairs or does it allow significantly non-planar structures as well? A positive answer to the question may lead to transition from the “planar approach” to the “stereo approach” that rely on the primary structure as the main source of an arbitrary secondary structure. Consequentially, it would allow the creation of more compact nanobiotechnological devices.

In our study [10], we prove that the model heteroassociates of the $m^1\text{Cyt} \cdot m^1\text{Thy}$ are capable of forming up

to ten observable molecular complexes. The first three of them have population of $\sim 90\%$ at standard conditions and are highly non-planar. The most energetically favorable structure has a T-shape, and the next two are of L-shape. Unfortunately, we failed to find any available published experimental data covering the self-assembly of the cytosine-thymine base pairs.

Presentation of the Hypothesis

As it was mentioned above, the modern nanobiotechnology constrains itself by the use of only planar nucleobase pairs. In our opinion, it results from a relative impossibility to produce stable non-planar nucleobase pairs, so

Table 1 Common physico-chemical properties of observable heteroassociates of the $m^1\text{Cyt} \cdot m^1\text{Thy}$

Complex	ΔG^0 , kcal/mol	μ , D	H-bond AH...B/vdW cont. A...B	ρ , a.u.	$\Delta\rho$, a.u.	100ε	d_{AB} , Å	d_{HB} , Å	Δd_{AH} , Å	$\angle AHB$, deg	E_{HB} , kcal/mol
1	0.00	5.22	N3...C4	0.007	0.024	37.6	3.197	–	–	–	1.19
			N4H...O4	0.021	0.078	7.6	2.997	1.991	0.010	169.3	3.87
			O2...N1	0.005	0.018	68.2	3.329	–	–	–	1.05
			C1H...O2	0.007	0.024	14.0	3.410	2.597	0.000	130.6	1.33
2	0.08	5.58	C1H...N3	0.011	0.033	11.1	3.340	2.488	–0.002	134.1	1.81
			N4H...O2	0.021	0.080	7.4	2.983	1.987	0.010	166.3	3.79
			O2...C6	0.002	0.008	101.0	3.716	–	–	–	0.34
3	0.17	5.65	N3...N1	0.006	0.020	110.8	3.314	–	–	–	1.16
			C1H...O2	0.008	0.023	8.7	3.554	2.584	–0.002	147.8	1.40
			N4H...O2	0.021	0.080	7.0	2.985	1.986	0.010	166.1	3.78
			C1H...N3	0.007	0.025	41.9	3.276	2.762	–0.002	108.5	1.30
4	0.82	2.91	N3H...N3	0.029	0.080	6.5	2.991	1.965	0.024	170.1	6.52
			N4H...O4	0.031	0.107	3.6	2.877	1.855	0.016	174.4	5.28
			O2...O2	0.002	0.008	23.1	3.714	–	–	–	0.33
5	1.23	2.06	N3H...N4	0.039	0.095	6.4	2.875	1.835	0.032	173.1	7.67
			N3H...O2	0.028	0.101	4.2	2.902	1.879	0.017	172.7	5.25
6	1.36	4.96	N3H...N3	0.029	0.079	6.4	2.995	1.969	0.023	169.9	6.40
			N4H...O2	0.028	0.101	4.0	2.901	1.883	0.014	173.2	4.85
			O2...O4	0.002	0.007	39.0	3.773	–	–	–	0.29
7	1.64	1.26	N3H...N4	0.040	0.096	6.4	2.865	1.823	0.033	173.6	7.86
			N3H...O4	0.030	0.103	3.5	2.889	1.863	0.019	173.2	5.61
8	1.95	5.06	C1H...N3	0.014	0.043	4.6	3.411	2.332	–0.001	169.5	2.28
			N4H...O2	0.022	0.089	6.5	2.962	1.948	0.010	174.2	3.70
9	2.22	13.05	C6H...O2	0.013	0.043	2.1	3.335	2.284	0.001	162.6	2.43
			C5-1H1..N3	0.004	0.012	0.2	4.047	2.978	0.000	166.2	0.66
			C1H...O2	0.008	0.030	15.5	3.488	2.449	–0.004	159.4	1.59
10	2.27	13.57	C1H...O2	0.005	0.017	173.4	3.798	2.814	–0.004	150.3	0.93
			C1H...N3	0.006	0.017	5.9	3.791	2.745	–0.004	161.1	0.95
			C6H...O2	0.014	0.051	1.4	3.294	2.211	0.001	175.5	2.65

ΔG^0 relative Gibbs free energy ($T = 298,15$ K; $P = 1$ atm), μ dipole moment, AH...B/A...B atoms participating in H-bond and/or in van der Waals contacts, ρ electron density, $\Delta\rho$ Laplacian of electron density, ε ellipticity in bond critical points of (3,-1) type, E_{HB} H-bond energy, d_{AB} , d_{HB} , $\angle AHB$ distances and angle between atoms of H-bond/van der Waals contact, Δd_{AH} elongation of AH group in H-bond

creation of some complex 3D structure out the innate planar elements requires usage of the sophisticated techniques. But if one were able to create the stable non-planar elements, achievement of the complex 3D structures might be much easier.

Taking into account the great conformational variety of the nucleobase pairs in the wild [9], as well as a relative lack of the theoretical awareness of all the possible conformations, we suppose that the nucleobase pairs are capable of forming observable non-planar structures. Because of a quite good knowledge of the complementary base pairs, we believe that those structures could be found in the non-canonical non-complementary nucleobase pairs. Additionally, we needed a means to find all possible conformations of the given nucleobase pairs. We solved that problem in [11].

Testing the Hypothesis

Our hypothesis would be successful if we could find some theoretical grounds for any observable non-planar nucleobase pair that have not been revealed by the previous base-pairing experiments. And this paper testifies that we managed to find such a pair. The more important fact is that it has not been found experimentally yet.

The main goal of this paper is to obtain all possible observable $m^1\text{Cyt} \cdot m^1\text{Thy}$ heteroassociates for answering the question in the title. To fulfill this task, we used our own algorithm [11] of the input structures creating. We would like to emphasize the importance of the algorithm, which basically proceeds from an assumption that the nucleobase pairs could be stabilized by at least two intermolecular H-bonds. Aside from this assumption, the algorithm has no other restrictions and uses a modern view of the chemical nature of the H-bonds [12]. As a result, we obtained numerous optimized and stable non-planar structures of both the canonical and non-canonical nucleobase pairs. Although most of them are highly energetic complexes in the free form, we can use

them for creating conditions in a crystal to achieve the exact desirable non-planar structure through restriction of the molecular degrees of freedom. That is how the wild-type RNA non-planar structures are created.

All the calculations have been carried out with the Gaussian 09 suite of the programs [13]. The relaxed geometries and their corresponding harmonic vibrational frequencies of the base pairs have been obtained using the density functional theory (DFT) with the B3LYP hybrid functional [14] for Pople's 6-311++G(d,p) basis set in a vacuum. We performed the single-point energy calculations at the correlated MP2 level of theory [15] with the 6-311++G(2df,pd) Pople's [16–18] basis set for B3LYP/6-311++G(d,p) geometries to consider the electronic correlation effects as accurately as possible.

The Gibbs free energy G values for all the structures were obtained at a room temperature ($T = 298.15$ K) in the following way:

$$G = E_{\text{el}} + E_{\text{corr}}, \quad (1)$$

where E_{el} is the electronic energy and E_{corr} is the thermal correction.

Bader's quantum theory "atoms in molecules" (QTAIM) was applied to analyze the electron density [19]. The topology of the electron density was examined using the program package AIMAll [20] with all the default options. The wave functions were obtained at the B3LYP/6-311++G(d,p) level of the theory. The presence of a bond critical point (BCP) of (3,-1) type [19] and a bond path between hydrogen donor and acceptor, as well as the positive value of the Laplacian at this BCP ($\Delta\rho \geq 0$), was considered as three criteria for the H-bond formation [19, 21].

Energies of the classical intermolecular H-bonds in base pairs were evaluated by the empirical Iogansen's formula [22]:

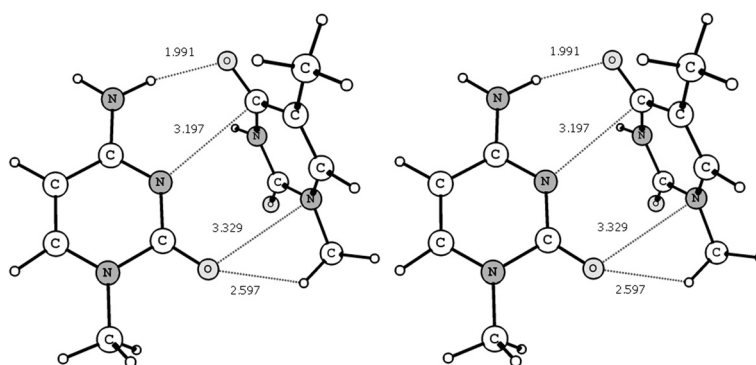


Fig. 1 Stereo image of the most energetically favorable heteroassociate of $m^1\text{Cyt} \cdot m^1\text{Thy}$. Its T-shaped and stabilized by means of two H-bonds and two van der Waals contacts (represented by dotted line; their corresponding bond lengths H...B/A...B are given in Å). Note that the 1-methyl group of $m^1\text{Thy}$ actively interacts with the $m^1\text{Cyt}$

$$E_{HB} = 0.33 \cdot \sqrt{\Delta\nu - 40}, \quad (2)$$

where $\Delta\nu$ is the magnitude of the redshift (relative to the free molecule) of the stretching mode of the H-bonded groups involved in the H-bonding. The partial

deuteration, namely the partial deuteration of the amino group, was applied to eliminate the effect of the vibrational resonances [23].

Energies of the non-canonical so-called weak intermolecular CH...O/N H-bonds were evaluated by the empirical

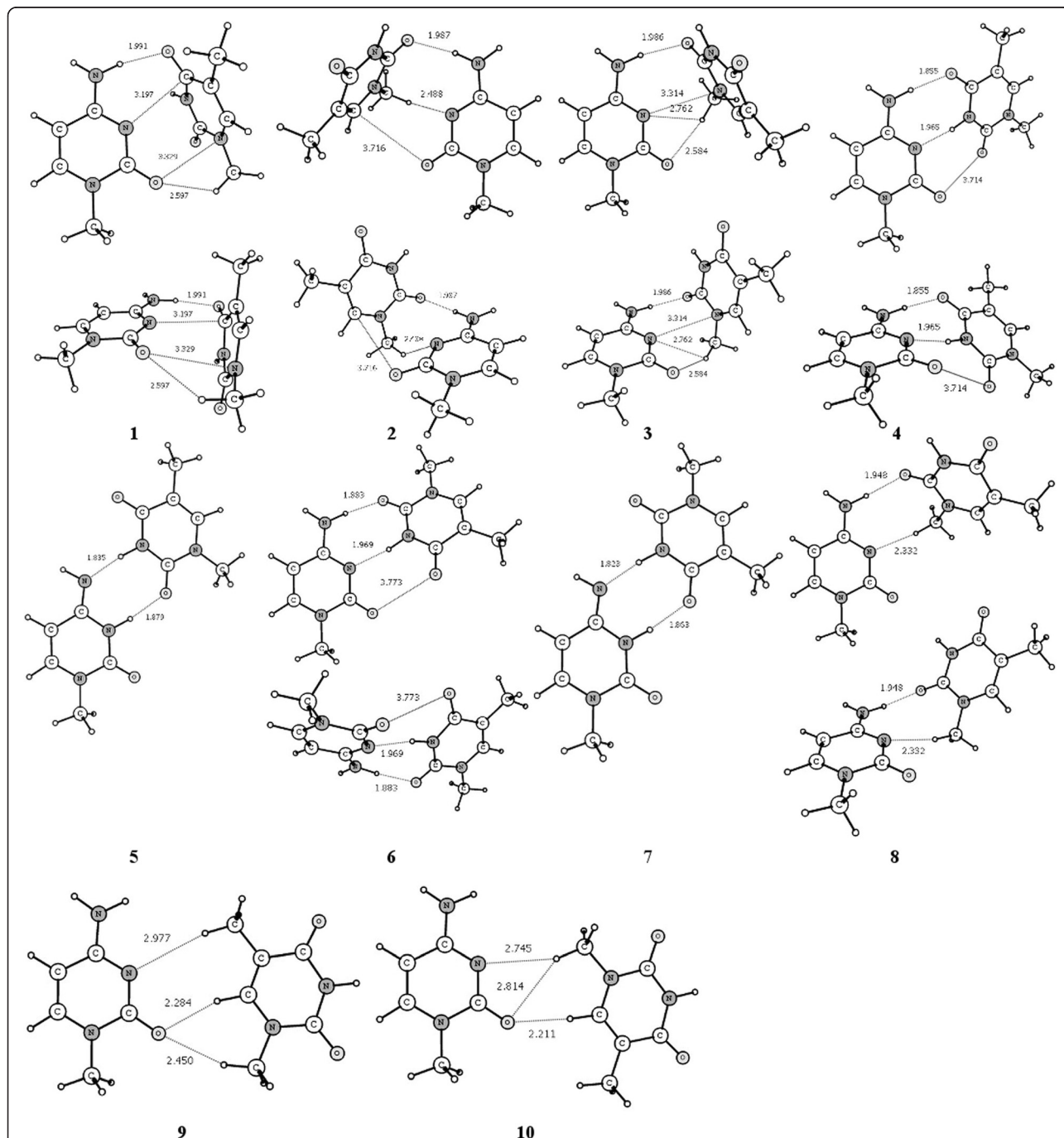


Fig. 2 Geometrical structure of observable at normal conditions heteroassociates of the $m^1\text{Cyt} \cdot m^1\text{Thy}$. The non-planar heteroassociates are represented in two projections while the planar ones are represented by one projection. Numbers under heteroassociates correspond to the row 'complex' of Table 1. H-bonds and van der Waals contacts (represented by dotted lines and their corresponding bond lengths H...B/A...B are given in Å)

Espinosa-Molins-Lecomte (EML) formula [24, 25] based on the electron density distribution at the (3,-1) BCPs of the H-bonds:

$$E_{\text{HB}} = 0.5 \times V(r), \quad (3)$$

where $V(r)$ is the value of a local potential energy at the (3,-1) BCPs.

Relative strengths of van der Waals contacts were estimated by means of Grunenberg's compliance constant formalism [26–28], calculated by the Compliance 3.0.2 program.

The main advantage of this approach is invariance of the compliance constants. The physical meaning of the compliance constants is deduced from their definition as a partial second derivative of the potential energy due to an external force:

$$C_{ij} = \frac{\partial^2 E}{\partial f_i \partial f_j}, \quad (4)$$

In other words, the compliance constants measure the displacement of an internal coordinate, resulting from a unit force acting on it. As follows from this definition, a lower numerical value of compliance constant corresponds to a stronger bond.

To study the charge transfer property in the interacting orbitals of the non-canonical intermolecular CH...O/N contacts, we used a natural bond orbital (NBO) analysis [29], which interprets the electronic wave function in terms of a set of occupied Lewis and a set of unoccupied non-Lewis localized orbitals. A second-order Fock matrix analysis was carried out to evaluate interactions between donor (i) and acceptor (j) bonds. The result of such interaction is a migration of the electron density from the idealized Lewis structure into an empty non-Lewis orbital σ^* . For each donor (i) and acceptor (j) bond, the stabilization energy is

$$E^{(2)} = \Delta E_{ij} = q_{ij} \frac{F(i,j)^2}{\varepsilon_j - \varepsilon_i}, \quad (5)$$

where q_i is the donor orbital occupancy, ε_j and ε_i are the diagonal elements, and $F(i,j)$ is the off diagonal element of the NBO Fock matrix.

The atomic numbering scheme for nucleobases is conventional [30].

Implications of the Hypothesis

We obtained the set of 51 complexes of the heteroassociates of $m^1\text{Cyt} \cdot m^1\text{Thy}$. This set contains both the common and the rare tautomeric forms.

Total occupancy of the obtained complexes **1** (30.50 %) + **2** (26.66 %) + **3** (22.90 %) + **4** (7.64 %) + **5** (3.80 %) + **6** (3.09 %) + **7** (1.93 %) + **8** (1.14 %) + **9** (0.72 %) + **10** (0.67 %) constitute 99.04 % at normal

conditions and defines all the experimentally observable complexes (see Table 1). For the purpose of achieving the declared goal, we will focus on these ten complexes in the rest of this paper.

The most energetically favorable complex **1** has a T-shape structure and is stabilized by means of two intermolecular H-bonds and two attractive van der Waals contacts (see Fig. 1).

We have found out that the obtained heteroassociates of the $m^1\text{Cyt} \cdot m^1\text{Thy}$ are stabilized by means of the intermolecular H-bonds of NH...N/O, CH...N/O types and attractive van der Waals contacts of the N...N/O/C, O...O/C. Energies of the classical H-bonds lie in diapason of 3.70 ÷ 7.86 kcal/mol. Energies of the non-canonical H-bonds lie in diapason of 0.66 ÷ 2.65 kcal/mol.

The observable heteroassociates of the $m^1\text{Cyt} \cdot m^1\text{Thy}$ have several different shapes (see Fig. 2): the T-shape is represented exclusively by the most energetically favorable complex **1**, an L-shape (complexes **2**, **3**), a spiral shape (complexes **4**, **6**), the planar structures (complexes **5**, **7**, **9**, **10**), and a severely non-planar structure of the complex **8** which cannot be classified as one of above. As one can see, the most expected shapes are the L-shape (49.56 %), the T-shape (30.5 %), the spiral shape (10.73 %), the planar shape (7.3 %), and finally the complex **8** shape (1.14 %). This fact gives us the positive answer to the question in the title.

We believe that such unusual geometries are the result of a strong involvement of a methyl group in stabilization of the heteroassociates. As one can see from Table 1, the methyl groups (C1H, C5H) are capable of forming the strong enough CH...O/N H-bonds with energies in diapason of 0.66 ÷ 2.28 kcal/mol. At the same time, one can observe the strong stabilizing van der Waals contacts (see Table 2), which are present in five

Table 2 Intermolecular CH...O/N H-bonds and van der Waals contacts in the observable heteroassociates of the $m^1\text{Cyt} \cdot m^1\text{Thy}$

Complex	H-bond/vdW contact AH...B/A..B	$E^{(2)}$, kcal/mol	Cstr, Å/mDyn
1	C1H...O2	0.36	39.549
2	C1H...N3	1.00	22.928
3	C1H...O2	0.76	37.566
	C1H...N3	0.03	33.407
8	C1H...N3	3.53	11.200
9	C6H...O2	3.27	16.085
	C5H...N3	0.55	66.521
	C1H...O2	1.00	27.809
10	C1H...O2	0.29	126.112
	C1H...N3	0.74	43.476
	C6H...O2	3.98	11.659

$E^{(2)}$ value of stabilization energy, Cstr linear Grunenberg constant

out of ten observable heteroassociates, and have energies in the diapason of $0.29 \div 1.19$ kcal/mol. The especially strong van der Waals contacts are surveyed in the most energetically favorable complex **1** with the energies of 1.05 and 1.19 kcal/mol respectively.

In our opinion, the experiment will show plenty of the mixed L-shapes and T-shapes, with quite rare inclusions of the spiral and planar shapes. This in turn presents a possibility of a self-assembly of a layered structure upon the self-assembled non-planar structures. This hypothesis will be tested in our future study.

For the first time, from the first principles, we show that the conformational capacity of the nucleic base pairs is much richer from the perspective of the self-assembly than it is used to consider in the modern nanobiotechnology. The capability of the modified cytosine and the modified thymine to create the significantly non-planar structures opens the way for the novel “stereo approach” to construction of the nanobiotechnological devices. We believe that the modern nanobiotechnological basis can and should be enriched by the new nucleic base pairs with an innate ability for the non-planar structures.

We think there might be at least three possible ways of a future development of the “stereo approach”.

The first way is to find the other non-planar nucleobase pairs that would be much more convenient for usage in a real industry than those that we have found and presented in this paper. The next way might be searching for an appropriate nucleobase modification in order to achieve the same goal. And the third way is to try to synthesize similar to the non-planar nucleobase pair structures which would behave themselves both as non-planar and energetically favorable at the same time.

Abbreviations

AIM: atoms in molecules; BCP: bond critical point; DFT: density functional theory; DNA: deoxyribonucleic acid; m¹Cyt: 1-methylcytosine; m¹Thy: 1-methylthymine; NBO: natural bond orbital; QTAIM: quantum theory: atoms in molecules; RNA: ribonucleic acid.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

AN carried out all the calculations in this paper and wrote the text of the paper. DM supervised the research project and reviewed and edited the manuscript. All authors contributed to the design of the study. Both authors read and approved the final manuscript.

Authors' information

DM has a degree of Doctor of Science in the field of Biology and he is a Corresponding Member of National Academy of Sciences (NAS) of Ukraine. Currently, DM holds the position of the Head of Department of Molecular and Quantum Biophysics of Institute of Molecular Biology and Genetics of NAS of Ukraine; he is a professor of the Department of Molecular Biology, Biotechnology and Biophysics of the Institute of High Technologies of Taras Shevchenko National University of Kyiv. DM authored more than 300 papers. His scientific interests cover quantum biology in general and the molecular mechanisms of point mutations in DNA. AN holds a degree of Master of Science in the field of Physics and occupies the position of a junior researcher in the Department of Molecular and

Quantum Biophysics of the Institute of Molecular Biology and Genetics of NAS of Ukraine. Also, AN is a PhD student in the Department of Molecular Biology, Biotechnology and Biophysics of the Institute of High Technologies of Taras Shevchenko National University of Kyiv.

Acknowledgements

This work was supported by the grant of the President of Ukraine to support scientific research of young scientists for the year 2015 from the State Fund for Fundamental Research of Ukraine (project no.GP/F61/028) and by the Grant of the NAS of Ukraine for young scientists for years 2015–2016.

Received: 24 November 2015 Accepted: 1 March 2016

Published online: 09 March 2016

References

- Rothemund PW (2006) Folding DNA to create nanoscale shapes and patterns. *Nature*; doi: 10.1038/nature04586
- Geary C, Rothemund PW, Andersen ES (2014) A single-stranded architecture for cotranscriptional folding of RNA nanostructures. *Science*; doi: 10.1126/science.1253920
- Wei B, Dai M, Yin P (2012) Complex shapes self-assembled from single-stranded DNA tiles. *Nature*; doi:10.1038/nature11075
- Endo M, Yamamoto S, Emura T, Hidaka K, Morone N, Heuser JE, Sugiyama H (2014) Helical DNA origami tubular structures with various sizes and arrangements. *Angew Chem Int Ed Engl*; doi: 10.1002/ange.201402973
- Yamazaki T, Heddle JG, Kuzuya A, Komiyama M (2014) Orthogonal enzyme arrays on a DNA origami scaffold bearing size-tunable wells. *Nanoscale*; doi: 10.1039/C4NR01598C
- Berman HM, Olson WK, Beveridge DL, Westbrook J, Gelbin A, Demeny T, Hsieh SH, Srinivasan AR, Schneider B (1992) The nucleic acid database. A comprehensive relational database of three-dimensional structures of nucleic acids. *Biophys J*; doi: 10.1016/S0006-3495(92)81649-1
- Narayanan BC, Westbrook J, Ghosh S, Petrov AI, Sweeney B, Zirbel CL, Leontis NB, Berman HM (2013) The nucleic acid database: new features and capabilities. *Nucl Acids Res*; doi: 10.1093/nar/gkt980
- Liu L, Xia D, Klausen LH, Dong M (2014) The self-assembled behaviour of DNA bases on the interface. *Int J Mol Sci*; doi: 10.3390/ijms15021901
- Chawla M, Oliva R, Bujnicki JM, Cavallo L (2015) An atlas of RNA base pairs involving modified nucleobases with optimal geometries and accurate energies. *Nucl Acids Res*; doi: 10.1093/nar/gkv606
- Glushenkov AN, Hovorun DN (2014) Confined set of H-bonded heteroassociates of m¹Cyt · m¹Thy: quantum-mechanical study. *Ukr Bioorg Acta* 12:1–3
- Glushenkov AN, Hovorun DM (2014) Geometric construction of all possible H-bonded associated nucleic base pairs. *Repts Natl Acad Sci Ukr* 8:133
- Steiner T (2002) The hydrogen bond in the solid state. *Angew Chem Int Ed*; doi: 10.1002/1521-3773(20020104)41:1 < 48:AID-ANIE48 > 3.0.CO;2-U
- Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA, Peralta JE, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Keith T, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas O, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ (2010) Gaussian 09, revision B.01. Gaussian, Inc, Wallingford
- Tirado-Rives J, Jorgensen WL (2008) Performance of B3LYP density functional methods for a large set of organic molecules. *J Chem Theory Comput*; doi: 10.1021/ct700248k
- Frisch MJ, Head-Gordon M, Pople JA (1990) Semi-direct algorithms for the MP2 energy and gradient. *Chem Phys Lett*; doi: 10.1016/0009-2614(90)80030-H
- Frisch MJ, Pople JA, Binkley JS (1984) Self-consistent molecular orbital methods 25. Supplementary functions for Gaussian basis sets. *J Chem Phys*; doi: 10.1063/1.447079
- Hariharan PC, Pople JA (1973) The influence of polarization functions on molecular orbital hydrogenation energies. *Theor Chem Acta* 28:3–213

18. Krishnan R, Binkley JS, Seeger R, Pople JA (1980) Self-consistent molecular orbital methods. XX. A basis set for correlated wave functions. *J Chem Phys*; doi: 10.1063/1.438955
19. Bader RFW (1990) *Atoms in molecules: a quantum theory*. Oxford University Press, Oxford
20. Keith TA (2011) AIMAll (Version 11.12.19). TK Gristmill Software, Overland Park, <http://aim.tkgristmill.com>. Accessed 07 Mar 2011.
21. Koch U, Popelier PLA (1995) Characterization of C-H-O hydrogen bonds on the basis of the charge density. *J Phys Chem*; doi: 10.1021/j100024a016
22. logansen AV (1999) Direct proportionality of the hydrogen bonding energy and the intensification of the stretching $\nu(\text{XH})$ vibration in infrared spectra. *Spectrochim. Acta Part A Mol Biomol Spectrosc*; doi: 10.1016/S1386-1425(98)00348-5
23. Yurenko YP, Zhurakivsky RO, Samijlenko SP, Ghomi M, Hovorun DM (2007) The whole of intermolecular H-bonding in the isolated DNA nucleoside thymidine. AIM electron density topological study. *Chem Phys Lett*; doi: 10.1016/j.cplett.2007.09.008
24. Espinosa E, Molins E, Lecomte C (1998) Hydrogen bond strengths revealed by topological analyses of experimentally observed electron densities. *Chem Phys Lett*; doi: 10.1016/S0009-2614(98)00036-0
25. Mata I, Alkorta I, Espinosa E, Molins E (2011) Relationships between interaction energy, intermolecular distance and electron density properties in hydrogen bonded complexes under external electric fields. *Chem Phys Lett*; doi: 10.1016/j.cplett.2011.03.055
26. Brandhorst K, Grunenberg J (2010) Efficient computation of compliance matrices in redundant internal coordinates from Cartesian Hessians for nonstationary points. *J Chem Phys*; doi: 10.1063/1.3413528
27. Brandhorst K, Grunenberg J (2008) How strong is it? The interpretation of force and compliance constants as bond strength descriptors. *Chem Soc Rev*; doi: 10.1039/B717781J
28. Grunenberg J, Barone G (2013) Are compliance constants ill-defined descriptors for weak interactions? *RSC Adv*; doi: 10.1039/C3RA22866E
29. Weinhold F, Landis C (2005) *Valency and bonding. A natural bond orbital donor-acceptor perspective*. Cambridge University Press, Cambridge
30. Saenger W (1984) *Principles of nucleic acid structure*. Springer, New York

Submit your manuscript to a SpringerOpen[®] journal and benefit from:

- Convenient online submission
- Rigorous peer review
- Immediate publication on acceptance
- Open access: articles freely available online
- High visibility within the field
- Retaining the copyright to your article

Submit your next manuscript at ► springeropen.com
