- The use of pedal taps or faucets automatic water supply in areas where we are working with radioactive substances;
- Drainage system drains to special sewerage from the rooms of premises and second zones;
- Alarm of overflow of decanter tanks of special sewerage;
- Floor and basement walls made of reinforced concrete.

To prevent accidents due to loss of ionizing radiation sources (IRS), the project envisages a system of lock and alarm facilities, which are stored the IRS, that will prevent the unauthorized access to IRS.

Also, PET-center is planned to organize security system, which should ensure the physical protection of the object (prevent accidental penetration of the public or third party personnel to the controlled area).

Conclusions Thus, basing on the results of environmental impact assessment of PET-center operation during normal mode and under emergency situations, it can be concluded that the risks arising from radiation influence on the environment and the population are within acceptable limit. At the same time the influence of construction of state-of-the-art medical center on the social environment will be positive.

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ОЦІНКА ВПЛИВУ НА ДОВКІЛЛЯ ЕКСПЛУАТАЦІЇ ЦЕНТРА ПОЗИТРОННО-ЕМІСІЙНОЇ ТОМОГРАФІЇ

Проведено аналіз впливу експлуатації центру позитронно-емісійної томографії на навколишнє природне середовище за рахунок радіаційних факторів. Показано, що в умовах нормального режиму експлуатації, а також при проектних і запроектних аваріях ризики, обумовлені цим впливом, знаходяться в межах прийнятних. Проаналізовано достатність захисних заходів для забезпечення радіаційної безпеки персоналу, населення і довкілля.

Ключові слова: *фтордеоксиглюкоза, медичний циклотрон, радіонукліди, радіоактивні газо-аерозольні викиди, радіоактивні відходи*

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ОЦЕНКА ВОЗДЕЙСТВИЯ НА ОКРУЖАЮЩУЮ СРЕДУ ЭКСПЛУАТАЦИИ ЦЕНТРА ПОЗИТРОННО-ЭМИСИОННОЙ ТОМОГРАФИИ

Проведен анализ воздействия эксплуатации центра позитронно-эмисионной томографии на окружающую среду за счет радиационных факторов. Показано, что в условиях нормального режима эксплуатации, а также при проектних и запроектных авариях риски, обусловленные этим воздействием, находятся в пределах приемлемых. Проанализировано достаточность защитных мер для обеспечения радиационной безопасности персонала, населения и окружающей среды

Ключевые слова: *фтордеоксиглюкоза, медицинский циклотрон, радионуклиды, радиоактивные газо-аэрозольные выбросы, радиоактивные отходы.*

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COMPLETE FAMILY OF H-BONDED 1-METHYLCYTOSINE HOMOASSOCIATES: QUANTUM-MECHANICAL INVESTIGATION

On the MP2/6-311++G(2df,pd)//B3LYP/6-311++G(d,p) theory level in vacuum for the first time was shown that stabilized by specific intermolecular contacts complete family of $m^1Cyt \cdot m^1Cyt$ homoassociates counts 37 structures in diapason of 0÷34,42 kcal/mol relative Gibbs energies. Centrally symmetric homoassociate corresponds to global minima which is stabilized by pair of antiparallel H-bonds N4H...N1 and has enthalpy of formation practically the same as in mass-spectrometry experiment (L.F. Sukhodub et al., 1976). Detail analysis of intermolecular H-bonds, especially weak CH...O/N, physico-chemical properties has been performed. Briefly discussed application of results in spontaneous point mutations of DNA theory.

Keywords: *nucleic base, nucleic bases pair, complete family, hydrogen bond, cytosine, methyl-, methyl group.*

Introduction. Nucleic bases (NB) play major role in coding genetic information, RNA spatial structure, engineering synthetic DNA. It's generally known that DNA strands hold complementary NB pairs of Gua·Cyt and Ade·Thy [23]. The complimentary principle is key factor supplying the transmission of genetic information in heredity line. Point changes of NB – mutations are possible through creation of incorrect pairs by rare NB tautomeric forms [24] which in turn leads to transformation of canonical NB pairs into non-canonical and errors during biosynthesis of DNA. RNA spatial structure in many respects is defined by intermolecular H-bonds between NB. Special emphasis in literature gives attention to non-canonical NB pairs in RNA [10–12, 20]. At the same time synthetic DNA can be designed to have non-canonical NB pairs. Every mentioned aspect demands knowledge about geometrical and physico-chemical properties of isolated NB as well as of their H-bonded associates.

Object and methods. The goal of this paper is to obtain geometrical and physico-chemical properties of all possible 1-methylcytosine (m^1Cyt) homoassociates which involve all of it's seven possible tautomeric forms. Input structures automatically generated by original algorithm. Geometrical and electronic structure of molecules and complexes as well as their wavefunctions were obtained using density functional theory on B3LYP/6-311++G(d,p) theory level in vacuum. All optimized structures has been checked on stability by absence of imaginary frequencies in their spectra. Electronic energies of NB interaction and NB Gibbs free energies were obtained on MP2/6-311++G(2df,pd)//B3LYP/6-311++G(d,p) theory level. Quantum-mechanical calculations were done in Gaussian 03 for Win32 application [9].

Intermolecular H-bond identification were done by QTAIM method [2]. For identification of CH..O/N H-bonds NBO-analysis [5] and Grunenberg constant [14,15] methods were additionaly used. Grunenberg constants calculations were done in Compliance 3.0.2 application [8]. Classical H-bond energies were calculated by Iogansen method [4,19]. Non-canonical CH..O/N H-bond energies and van-der-Waals contacts were calculated by Espinosa-Mollins-Lecomte method (EML) [18].

Results and discussion.

Fundamental physico-chemical properties of m^1Cyt·m^1Cyt homoassociates. Results are presented in table 1. Atomic numbering based on standard scheme [3]. Belonging to the same plane as molecule methyl group hydrogen atom has index 1. Complete family of H-bonded homoassociates m^1Cyt·m^1Cyt contains 37 structures. These structures consists of NB pairs in common tautomeric form as well as rare tautomeric forms. Most energetically favorable conformer **1** has centrosymmetrical structure, stabilized by two antiparallel H-bonds on m^1Cyt Watson-Crick binding site (naming convention by [21]) and has zero dipole moment. Ten homoassociates m^1Cyt·m^1Cyt has planesymmetrical structure (3 of them are centrosymmetrical); other 27 are significantly non-planar.

Conformer **1**'s population in standard conditions is 99,97% and conformers **2**, **3** has total population of ~0,03%.

It was established that homoassociates m^1Cyt·m^1Cyt are stabilized by bond types: NH...N; NH...O; OH...N; OH...O; CH...N; CH...O. Classic H-bond energies lie in diapason 0,39÷2,80 kcal/mol (table 1).

***Table* 1a**

Fundamental physicochemical properties of m^1Cyt·m^1Cyt homoassociates

Complex	ΔG^0, kcal/mol	μ, D	H-bond/vdW contact AH...B /A...B	ρ, a.u.	Δρ, a.u.	100ε	E_{HB}, kcal/mol
1	0.00	0.00	N4H1...N3	0.032	0.088	0.08	6.39
			N4H1...N3	0.032	0.088	0.08	6.39
2	5.31	6.54	N3H...N3	0.028	0.080	0.07	5.90
			N4H...O2	0.016	0.054	0.02	3.11
			N4H1...O2	0.031	0.031	0.05	5.42
3	5.49	4.79	N3...C2	0.007	0.024	139.4	1.22
			N4H1...N3	0.020	0.063	0.05	4.20
			C1H...O2	0.002	0.009	0.41	0.39
4	6.47	2.99	C1H...N3	0.014	0.041	0.05	2.19
			N4H1...O2	0.027	0.105	0.06	4.67
5	6.64	13.38	N4H2...O2	0.025	0.088	0.06	4.16
6	7.48	14.93	C5H...N3	0.006	0.017	0.05	0.96
			N4H2...O2	0.024	0.089	0.04	4.06
7	7.54	10.60	N4H2...N3	0.022	0.068	0.02	4.71
			N4H1...N4	0.014	0.044	0.12	2.63
8	7.81	13.28	N4H2...N3	0.019	0.060	0.08	3.67
			C5H...O2	0.009	0.030	0.04	1.69
9	7.85	10.64	C6H...O2	0.012	0.037	0.03	2.14
			C1H1...O2	0.006	0.019	0.23	1.15
10	8.01	1.00	N1...O2	0.004	0.017	170.5	0.92
			C1H...O2	0.008	0.025	0.13	1.44
			O2...N1	0.005	0.018	232.2	1.02
			C1H...O2	0.006	0.022	0.38	1.24
			C1H...N3	0.006	0.018	0.70	0.99
11	8.16	5.54	N3...C5	0.005	0.014	109.4	0.72
			N4H1...N4	0.011	0.033	0.04	2.22
			C1H...O2	0.007	0.022	0.20	1.28
12	8.82	12.25	C6H...O2	0.013	0.042	0.04	2.35
			C1H1...O2	0.007	0.021	0.22	1.28
13	8.83	3.99	N3H...N3	0.029	0.080	5.81	6.76
			N4H1...N4	0.033	0.088	5.46	6.75
			O2...O2	0.002	0.002	4.74	0.34
14	8.97	13.90	C6H...O2	0.014	0.045	0.03	2.50
			C1H1...O2	0.008	0.025	0.20	1.43

Table 1a (*Continue*)

Complex	ΔG^0, kcal/mol	μ, D	H-bond/vdW contact AH...B /A...B	ρ, a.u.	Δρ, a.u.	100ε	E_{HB}, kcal/mol
15	9.52	12.69	C6H...O2	0.015	0.052	0.04	2.80
			C1H1...N3	0.006	0.016	0.02	0.89
16	9.75	0.41	N3H...O2	0.027	0.100	3.38	5.22
			N3H...N4	0.037	0.092	5.44	7.48
17	10.16	6.31	N4H...N3	0.019	0.060	0.05	2.45
			N3H...O2	0.023	0.082	0.05	3.77
18	10.30	4.86	C5H...N3	0.017	0.052	0.07	1.96
			N4H1...N4	0.028	0.080	0.08	5.91
19	10.37	5.28	C1H...O2	0.013	0.045	0.07	2.41
			C1H...O2	0.013	0.044	0.07	2.36
20	10.63	3.89	N4H1...O2	0.028	0.101	0.04	4.85
			N3H...N3	0.027	0.077	0.06	6.13
			O2...N4	0.002	0.007	20.11	0.28
21	10.95	10.81	C5H...N3	0.010	0.030	0.09	1.58
			N4H2...N4	0.011	0.031	0.06	1.15
22	11.21	0.97	C1H...O2	0.013	0.043	0.07	2.34
			C1H...O2	0.013	0.043	0.07	2.32
23	11.48	4.05	C1H...O2	0.012	0.040	0.07	2.16
			C1H...O2	0.012	0.045	0.04	2.34
24	11.96	6.81	N4H2...N4	0.014	0.041	0.05	2.23
25	12.68	0.00	N3H...O2	0.026	0.097	0.03	4.70
			N3H...O2	0.026	0.097	0.03	4.70
26	16.62	1.30	N4H1...N3	0.038	0.098	0.07	6.98
			O2H...N3	0.058	0.093	0.06	10.72
27	17.70	4.89	O2H...N3	0.057	0.096	0.05	10.34
			N4H1...N3	0.035	0.090	0.07	6.90
28	21.55	3.42	C1H...N3	0.011	0.034	0.11	1.87
			O2H...O2	0.050	0.143	0.05	8.54
29	22.05	2.81	C1H...N3	0.010	0.026	0.05	1.49
			O2H...O2	0.047	0.146	0.05	7.77
30	22.54	6.82	N3H...N3	0.033	0.084	0.06	7.15
			N4H...N4	0.015	0.045	0.05	2.41
			O2H...O2	0.048	0.142	0.03	7.69
31	23.22	0.96	N3...N3	0.012	0.038	9.80	2.18
			O2H...O2	0.045	0.127	0.04	8.62
			N4H1...N4	0.027	0.076	0.08	6.78
32	23.53	4.34	N3H...N3	0.034	0.087	0.06	7.12
			O2H...N4	0.078	0.084	0.05	12.59
			N4...O2	0.002	0.008	8.96	0.39
33	28.30	4.17	N3H...N3	0.025	0.077	5.88	5.90
			N4...N4	0.002	0.006	9.11	0.29
			O2H...O2	0.050	0.128	1.53	8.33
34	29.70	12.35	C1H...O2	0.008	0.027	0.39	1.55
			C1H...O2	0.010	0.035	0.19	1.89
			O2H...O2	0.041	0.140	0.04	6.79
35	30.72	15.03	O2H...O2	0.039	0.126	0.05	6.87
			C1H...O2	0.011	0.038	0.23	2.10

Table 1a (*End*)

Complex	ΔG^0, kcal/mol	μ, D	H-bond/vdW contact AH...B /A...B	ρ, a.u.	Δρ, a.u.	100ε	E_{HB}, kcal/mol
36	31.68	0.06	O2H...N3	0.081	0.073	0.05	13.10
			O2H...N3	0.081	0.074	0.05	13.06
37	34.42	13.38	O2H...O2	0.039	0.125	0.05	6.80
			C1H...O2	0.010	0.037	0.24	2.00

Table 1b

Fundamental physicochemical properties of m^1Cyt·m^1Cyt homoassociates

Complex	H-bond/vdW contact AH...B /A...B	d_{AB}, Å	d_{HB}, Å	Δd_{AH}, Å	∠AHB, deg
1	N4H1...N3	2.946	1.917	0.023	175.7
	N4H1...N3	2.946	1.917	0.023	175.7
2	N3H...N3	3.005	1.977	0.020	174.6
	N4H...O2	3.187	2.164	0.004	177.8
	N4H1...O2	2.864	1.840	0.017	176.6
3	N3...C2	3.202	-	-	-
	N4H1...N3	3.096	2.110	0.012	161.8
	C1H...O2	3.794	3.289	0.000	109.5
4	C1H...N3	3.427	2.349	0.000	168.9
	N4H1...O2	2.888	1.867	0.014	176.3
5	N4H2...O2	2.970	1.953	0.011	179.8
6	C5H...N3	3.762	2.746	0.000	156.5
	N4H2...O2	2.967	1.952	0.011	176.0
7	N4H2...N3	3.032	2.109	0.015	149.5
	N4H1...N4	3.190	2.298	0.006	146.1
8	N4H2...N3	3.152	2.149	0.009	169.4
	C5H...O2	3.456	2.440	0.000	156.0
9	C6H...O2	3.372	2.345	0.000	157.3
	C1H1...O2	3.675	2.689	-0.002	150.4
10	N1...O2	3.360	-	-	-
	C1H...O2	3.403	2.599	0.000	129.9
	O2...N1	3.317	-	-	-
	C1H...O2	3.476	2.685	0.000	129.0
	C1H...N3	3.794	2.751	0.000	160.0
11	N3...C5	3.568	-	-	-
	N4H1...N4	3.416	2.408	0.005	172.7
	C1H...O2	3.368	2.659	0.000	122.2
12	C6H...O2	3.352	2.294	0.001	164.5
	C1H1...O2	3.637	2.621	-0.001	155.0
13	N3H...N3	2.977	1.946	0.025	173.0
	N4H1...N4	2.927	1.898	0.025	174.0
	O2...O2	3.701	-	-	-
14	C6H...O2	3.316	2.264	0.001	162.8
	C1H1...O2	3.552	2.527	-0.001	156.4
15	C6H...O2	3.277	2.201	0.001	171.0
	C1H1...N3	3.875	2.791	0.000	172.8
16	N3H...O2	2.902	1.879	0.017	172.5
	N3H...N4	2.883	1.846	0.030	172.5

Table 1b (*Continue*)

Complex	H-bond/vdW contact AH...B /A...B	d_{AB}, Å	d_{HB}, Å	Δd_{AH}, Å	∠AHB, deg
17	N4H...N3	3.185	2.170	0.002	171.7
	N3H...O2	3.001	1.978	0.014	176.4
18	C5H...N3	3.310	2.242	0.005	167.7
	N4H1...N4	3.008	1.981	0.020	176.4
19	C1H...O2	3.323	2.260	0.000	164.2
	C1H...O2	3.332	2.271	0.000	163.6
20	N4H1...O2	2.903	1.887	0.014	172.7
	N3H...N3	3.010	1.988	0.022	169.3
	O2...N4	3.862	-	-	-
21	C5H...N3	3.529	2.477	0.001	163.9
	N4H2...N4	3.437	2.429	0.002	178.3
22	C1H...O2	3.352	2.267	0.000	172.3
	C1H...O2	3.357	2.271	0.000	172.3
23	C1H...O2	3.340	2.311	-0.002	156.9
	C1H...O2	3.350	2.262	0.000	175.1
24	N4H2...N4	3.288	2.325	0.004	159.0
25	N3H...O2	2.913	1.903	0.014	167.2
	N3H...O2	2.913	1.904	0.014	167.2
26	N4H1...N3	2.868	1.843	0.027	170.1
	O2H...N3	2.689	1.667	0.057	175.3
27	O2H...N3	2.686	1.671	0.052	173.3
	N4H1...N3	2.923	1.894	0.026	173.0
28	C1H...N3	3.313	2.469	-0.002	133.4
	O2H...O2	2.630	1.627	0.036	177.5
29	C1H...N3	3.517	2.558	-0.001	146.3
	O2H...O2	2.637	1.640	0.029	176.2
30	N3H...N3	2.950	1.918	0.028	171.0
	N4H...N4	3.312	2.289	0.002	178.3
	O2H...O2	2.647	1.658	0.028	171.3
31	N3...N3	2.972	-	-	-
	O2H...O2	2.674	1.687	0.038	166.0
	N4H1...N4	3.019	1.988	0.027	173.2
32	N3H...N3	2.920	1.903	0.029	164.8
	O2H...N4	2.594	1.547	0.081	175.8
	N4...O2	3.733	-	-	-
33	N3H...N3	2.998	2.001	0.021	161.4
	N4...N4	3.948	-	-	-
	O2H...O2	2.631	1.631	0.034	175.2
34	C1H...O2	3.359	2.565	-0.002	129.0
	C1H...O2	3.308	2.421	-0.005	137.4
	O2H...O2	2.680	1.705	0.023	168.9
35	O2H...O2	2.720	1.746	0.024	168.5
	C1H...O2	3.278	2.379	-0.006	138.7
36	O2H...N3	2.591	1.534	0.089	179.2
	O2H...N3	2.594	1.537	0.089	179.5

Table 1b (*End*)

Complex	H-bond/vdW contact AH...B /A...B	d_{AB}, Å	d_{HB}, Å	Δd_{AH}, Å	∠AHB, deg
37	O2H...O2	2.723	1.750	0.024	168.1
	C1H...O2	3.294	2.396	-0.006	138.7

Note: ΔG^0 - relative Gibbs free energy (T=298,15K; P=1atm); μ — dipole moment; AH...B/A...B — atoms forming H-bond and/or van-der-Waals contact; ρ — electron density at BCP, Δρ — laplacian of electron density at the BCP, ε — ellipticity at the BCP; E_{HB} — H-bond energy; distances d_{AB}, d_{HB} and angle ∠AHB between H-bond atoms; elongation Δd_{AH} of H-bonded AH group

Identification of weak CH..O/N H-bonds. Weak CH..O and CH..N bonds attract special interest in literature. One of the problems discussed are their physicochemical properties and classification. It was established [17] that in such conditions that type of specific contacts is true H-bond. Our interest has been attracted to this H-bonds because 20 out 37 conformers in complete conformational family of $m^1Cyt{\cdot}m^1Cyt$ homoassociates are stabilized through CH..O/N H-bonds. In 16 conformers m-group in position 1 takes part in CH..O/N H-bonds as proton donor. As we can see from table 1 QTAIM method identifies all specific CH..O/N contacts as H-bond. Although for their robust identification as a true H-bonds we additionally used NBO-analysis [5] and Grunenberg constants methods [14,15].

Quantum-mechanical calculations' results of stabilization energies $E^{(2)}$ and Grunenberg constants for these H-bonds are presented in table 2. As we can see all values $E^{(2)}>0$ which means charge transfer from atom-acceptor lone pair to C-H antibond. Also all Grunenberg constants are positive which means stabilization (pull not push) nature of specific CH..O/N contacts. No charge transfer in complex 3 means borderline case of transformation H-bond into van-der-Waals contact and can be useful for future investigations of lower bounds for electron density and it's laplacian in corresponding H-bond critical point. Obviously, that by using QTAIM theory only, it's hard if not possible at all to tell the difference between AH..B H-bond and A..B van-der-Waals contact. It's seen from table 1 that for van-der-Waals contacts electron density values belong to 0.002-0.012 a.u. diapason and laplacian of electron density values belong to 0.006-0.038 a.u. diapason. At the same time for weak H-bonds electron density values belong to 0.006-0.019 a.u. and laplacian of electron density values belong to 0.009-0.052 a.u. Comparability of values in both cases shows us the necessity of QTAIM usage in pair with NBO-analysis for identification and investigation of weak H-bonds nature. Although this fact doesn't diminish the value of QTAIM analysis as most generic and relatively cheap method for modeling electronic clouds.

We'll add that for CH..O/N contacts we found linear relation of H-bond energy E_{HB} from electron density in bond critical point ρ. Relations for data in table 1 are $E_{HB}^{CH...O} = 175.121 \cdot \rho + 0.107$ and $E_{HB}^{CH...N} = 163.684 \cdot \rho - 0.044$ with RMSD values of 0.0003 kcal/mol and 0.0043 kcal/mol respectively. Data extrapolation on base of these relations to minimal electron density value of ρ=0,002 a.u. gives adequate minimal H-bond energy values of $E_{HB}^{CH...O}(\min) = 0,46 \text{kcal/mol}$ and $E_{HB}^{CH...N}(\min) = 0,28 \text{kcal/mol}$.

Table 2

Stabilization energies $E^{(2)}$ and linear Grunenberg constant Cstr values for intermolecular CH..O/N H-bonds in $m^1Cyt{\cdot}m^1Cyt$ homoassociates (calculations on B3LYP/6-311++G(d,p) theory level)

Complex	AH...B	$E^{(2)}$, kcal/mol	Cstr, Å/mdyn
3	C1H...O2	0.00	210.862
4	C1H...N3	3.32	11.904
6	C5H...N3	0.96	56.735
8	C5H...O2	1.79	35.720
9	C6H...O2	2.36	29.497
	C1H1...O2	0.37	66.103
10	C1H...O2	0.16	55.063
	C1H...O2	0.08	81.740
	C1H...N3	0.21	58.270
11	C1H...O2	0.06	233.045
12	C6H...O2	3.03	20.523
	C1H1...O2	0.42	71.288
14	C6H...O2	3.30	16.476
	C1H1...O2	0.60	42.019
15	C6H...O2	4.41	9.990
	C1H1...N3	0.89	49.176
18	C5H...N3	5.53	8.214
19	C1H...O2	1.66	14.329
	C1H...O2	1.62	15.430

Table 2 (*End*)

Complex	AH...B	$E^{(2)}$, kcal/mol	Cstr, Å/mdyn
21	C5H...N3	1.46	18.925
22	C1H...O2	1.41	14.395
	C1H...O2	1.35	14.539
23	C1H...O2	1.12	25.317
	C1H...O2	2.49	13.805
28	C1H...N3	0.90	17.845
29	C1H...N3	1.08	56.163
34	C1H...O2	0.51	30.099
	C1H...O2	0.75	24.909
35	C1H...O2	0.72	21.020
37	C1H...O2	0.71	21.897

Interpretation of classic mass-spectrometry experiment. In [1, 6, 7] is described mass-spectrometry experiment with registration of associating biomolecules in vacuum. In this experiment reaction $m^1Cyt + m^1Cyt \leftrightarrow m^1Cyt{\cdot}m^1Cyt$ has been registered and it's reported standard enthalpy of formation has value of ΔH = 73,3 kJ/mol for T=383K. Basing our hypothesis on population value of most energetically favorable homoassociate 1, we calculated for it standard enthalpy of formation with account of so-called BSSE correction. We report theoretical value of ΔH = 72,09 kJ/mol which coincides with experimental value with precision of 1.65%. This tells us that experimental value of standard enthalpy of formation corresponds to most energetically favorable complex 1 (table 1, pic. 1). By the way, exceptional coincidence of theoretical and experimental data which were obtained through extrapolation on zero field technique points on legitimacy of the last.

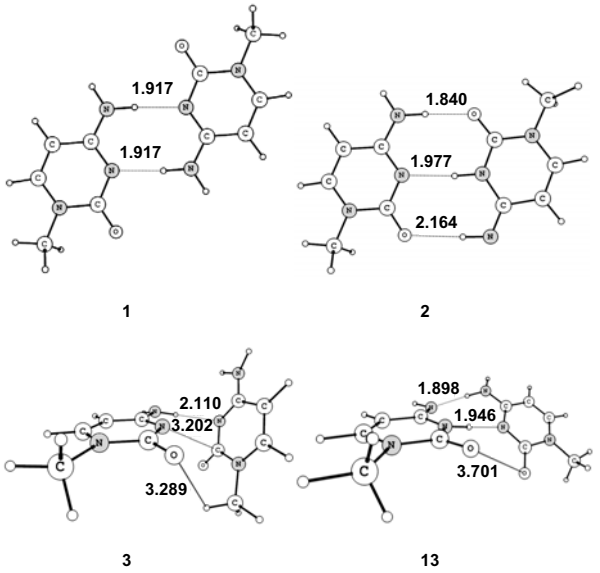

Fig. 1. Chosen m1Cyt·m1Cyt homoassociates (see also tables 1 and 2).
Intermolecular H-bonds and van-der-Waals contacts are depicted by dotted lines. Their distances H...B and A...B are shown in Å.

Spontaneous point mutations theory. Obtained data is also useful in spontaneous point mutations theory which is today far from it's complete and non-contradiction state. Such in paper [16] propeller-like homoassociate is postulated. It's so-called short Watson-Crick pair of Cyt·Cyt* which is stabilized by two H-bonds N3 H...N3, N4 H4-1...N4 and van-der-Waals contact O2..O2 and is transversion. Our data shows that this same complex is homoassociate 13 (ΔG^0=8,83 kcal/mol) and is most energetically favorable among all other homoassociates with syn-oriented glycosidic bonds N1–C1m. This fact strongly evidences against all other possible alternatives and pair of Cyt·Cyt* is responsible for spontaneous point mutations of this type during DNA biosynthesis.

Conclusions. First to obtain complete family of m1Cyt·m1Cyt homoassociates for standard conditions. Complete family contains 37 structures with relative Gibbs free energies in 0÷34,42 kcal/mol. Homoassociates are stabilized through classic (NH...N; NH...O; OH...N; OH...O) and weak (CH...N; CH...O) H-bonds as well as van-der-Waals contacts. It's shown that sugar-replacing methyl group is proton donor in H-bonds and influences Gibbs distribution for homoassociates. We show that QTAIM theory should be used in concert with NBO-analysis while investigating specific intermolecular contacts. Linear relation between CH..O/N H-bond energy EHB and electron density in bond critical point ρ. First to interpret theoretically result of classical mass-spectrometry experiment (L.F. Sukhodub et al., 1976). Showed theoretically that homoassociate m1Cyt·m1Cyt* is responsible for spontaneous point mutations during DNA biosynthesis.

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ПОВНЕ СІМЕЙСТВО Н-ЗВ'ЯЗАНИХ ГОМОАСОЦІАТІВ 1-МЕТИЛЦИТОЗИНУ: КВАНТОВО-МЕХАНІЧНЕ ДОСЛІДЖЕННЯ

На рівні квантово-механічної теорії MP2/6-311++G(2df,pd)//B3LYP/6-311++G(d,p) в вакуумному наближенні вперше показано, що повне сімейство гомоасоціатів $m^1Cyt{\cdot}m^1Cyt$, стабілізованих специфічними міжмолекулярними контактами за нормальних умов, нараховує 37 структур в діапазоні відносних енергій Гіббса 0÷34,42 ккал/моль. Глобальному мінімуму енергії відповідає центросиметричний гомоасоціат, стабілізований парою антипаралельних Н-зв'язків N4H...N1: ентальпія його утворення практично співпадає із результатами мас-спектрометричного експерименту (Л.Ф. Суходуба та ін., 1976). Детально проаналізовано основні фізико-хімічні властивості міжмолекулярних, особливо слабких CH...O/N, Н-зв'язків. Коротко обговорюється застосування отриманих результатів в теорії спонтанних точкових мутацій ДНК.

Ключові слова: *нуклеїнова основа, пара нуклеїнових основ, повне сімейство, водневий зв'язок, цитозин, метил-, метильна група.*

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ПОЛНОЕ СЕМЕЙСТВО Н-СВЯЗАННЫХ ГОМОАССОЦИАТОВ 1-МЕТИЛЦИТОЗИНА: КВАНТОВО-МЕХАНИЧЕСКОЕ ИССЛЕДОВАНИЕ

На уровне квантово-механической теории MP2/6-311++G(2df,pd)//B3LYP/6-311++G(d,p) в вакуумном приближении впервые показано, что полное семейство гомоассоциатов $m^1Cyt{\cdot}m^1Cyt$, стабилизируемых специфическими межмолекулярными контактами при нормальных условиях, насчитывает 37 структур в диапазоне относительных энергий Гиббса 0÷34,42 ккал/моль. Глобальному минимуму энергии соответствует центросимметричный гомоассоциат, стабилизирующийся парой антипараллельных Н-связей N4H...N1: энтальпия его образования практически совпадает с результатами масс-спектрометрического эксперимента (Л.Ф. Суходуба и др., 1976). Детально проанализированы основные физико-химические свойства межмолекулярных, особенно слабых CH...O/N, Н-связей. Кратко обсуждается применение полученных результатов в теории спонтанных точечных мутаций ДНК.

Ключевые слова: *основание нуклеиновой кислоты, пара нуклеиновых оснований, полное семейство, водородная связь, цитозин, метил-, метильная группа.*

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DEVELOPMENT AND TESTING OF THE EXPERIMENTAL SYSTEM FOR REGISTRATION OF FOOD REFLEX IN RATS

Automated system for registration of behavioural feeding response in rats designed and developed. The system includes the specialized hardware and software. The testing of the system is conducted.

Keywords: *cognitive abilities, food reflex, rat, photoelectric registration.*

Introduction. According to the World Health Organization, currently about 450 million people worldwide suffer from mental and neurological disorders, the most widespread are cognitive impairment. Among those it should be mentioned the diseases such as ischemia, Alzheimer's disease, Parkinson's disease, neuropathy and others [2]. However, the molecular mechanisms involved in the abnormal neurogenesis of various nervous diseases are not yet fully understood. In this connection, it is relevant to study the mechanisms of nervous diseases that are the basis of integrative brain function in the implementation of complex behaviors in normal and most common neurodegenerative pathologies. For recording of the changes in the functioning of the brain and cognitive abilities the study of complex behaviors in animals are used. The aim of given work was to create a registration system of food behavioral responses of rats for the automatic recording of the time characteristics of a conditioned reflex movements and manipulations of rat. Comparing the characteristics for control animals and animal model (with induced disease of the nervous system) makes it possible to evaluate objectively the disruption of the brain function during pathologies and to assess the cognitive abilities of experimental animals. This system