Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:

Tailoring the Properties of Quadruplex Nucleobases for Biological and Nanomaterial Applications

Jan Novotný,[a,b] Yevgen P. Yurenko,[a] Petr Kulhánek,[a,b] Radek Marek[a,b,c]*

[a] CEITEC – Central European Institute of Technology, Masaryk University, Kamenice 5/A4, Brno, CZ-625 00, Czech Republic

[b] National Center for Biomolecular Research, Faculty of Science, Masaryk University, Kamenice 5/A4, Brno, CZ-625 00, Czech Republic

[c] Department of Chemistry, Faculty of Science, Masaryk University, Kotlářská 267/2, Brno, CZ-611 37, Czech Republic

Stacking energy of guanine dimer – comparison of DFT-D3 and CCSD(T) values

Table S1. Interaction energies of stacked model of guanine pair (experimental geometry) obtained from S22 benchmark set[1] (values in kcal mol^{-1} calculated in vacuum without deformation energy).

Method	**G.G stack**
CCSD(T)/CBS	-12.67[1]
BLYP-D3/def2-TZVPP	-12.98
BLYP-D3-BJ/def2-TZVPP	-13.12
TPSS-D3/def2-TZVPP	-11.62

Preparation of models

The starting structures of guanine based systems were derived from the structure of tetramolecular parallel quadruplex[2,3] (PDB 139D) by deleting all atoms of backbone. To prepare models of assemblies comprised from xanthine derivatives, the original guanine structures were manually modified in program Chimera 1.5.[4]

All presented structures, unless otherwise stated, were fully optimized at RI-BLYP-D3 level of theory[5–9] using def2-TZVPP basis set[10] in Turbomole 6.3 program[11,12] using redundant internal coordinates (grid for integration m5, default set of auxiliary basis set (RI),[7,8] convergence criteria: energy 10^{-6}, Cartesian gradient 10^{-3}). The dispersion correction to energy (D3) was incorporated by Grimme's approach.[9] The effect of water solvent was included by COSMO[13] model (relative dielectric constant of environment 78.4, radius of solvent molecule 1.93 Å, default values of atomic radii). In the case of three stacked models $(B_4)_3$, the geometry was pre-optimized employing def2-SVP basis set in vacuum.

The formation energies in all calculations were obtained as a difference between the energy of optimized complex and separately optimized components in implicit solvent at the same level of theory that was used for geometry optimization (if not stated otherwise). Presented properties were also calculated at the same level of theory. VMD[14] or Chimera[4] software packages were employed for visualizing structures.

Table S2. Atomic charges for modified nucleobases derived from the electrostatic potential employing MK scheme.[15,16]

Base	O6	H1	O2	NH2	H7/N7
G	-0.6387	0.4153	-	0.4019	-0.7031
X	-0.6195	0.4038	-0.6618	-	0.4039
FdaX	-0.6437	0.3738	-0.6668	-	0.3909
CldaX	-0.6259	0.3677	-0.6681	-	0.3304
MX	-0.6389	0.4008	-0.6678	-	0.4019
AdaX	-0.6039	0.3525	-0.6594	-	0.2977

Table S3. Formation energies for selected systems. For the interaction of the cation with two-stacked system (B_8 + Na^+ or B_8 + K^+), the overall energy is expressed as a sum of electronic and desolvation contribution (all values are in kcal mol^{-1}).

Formation step	**X**	**FdaX**	**CldaX**	**G**
$4B \rightarrow B_4$	-30	-33	-33	-33
$B_4 + Na^+$	-25	-26	-26	-30
$2B_4 \rightarrow B_8$	-27	-31	-35	-22
$B_8 + Na^+$	-44 (-117+73)	-48	-48	-58 (-155+97)
$B_8 + K^+$	-42 (-98+56)	-46	-45	-55 (-135+80)
$3B_4 \rightarrow B_{12}$	-56	-61	-68	-40
$B_{12} + Na^+$	-49	-54	-52	-66
$B_{12} + K^+$	-45	-52	-53	-63
$B_{12} \cdot Na^+ + Na^+$	-35	-42	-40	-52
$B_{12} \cdot K^+ + K^+$	-29	-36	-37	-48

Systematic investigation of stacking interaction – twist-rise scan

The symmetric models of $(B_4)_2 \cdot M^+$ were created from two replicas of tetrads optimized by applying the C_{4h} symmetry in the *xy*-plane. The individual points of 2D potential energy surface were generated by incrementing the *z* coordinates (0.05 Å) and twist angle (5°) of one tetrad with respect to the second one. The cation was placed at the geometrical center of two stacked system. For each point, the single point energy was calculated and the result for $(G_4)_2 \cdot K^+$ is shown in Figure S1A and for $(FdaX_4)_2 \cdot K^+$ in Figure S1B.

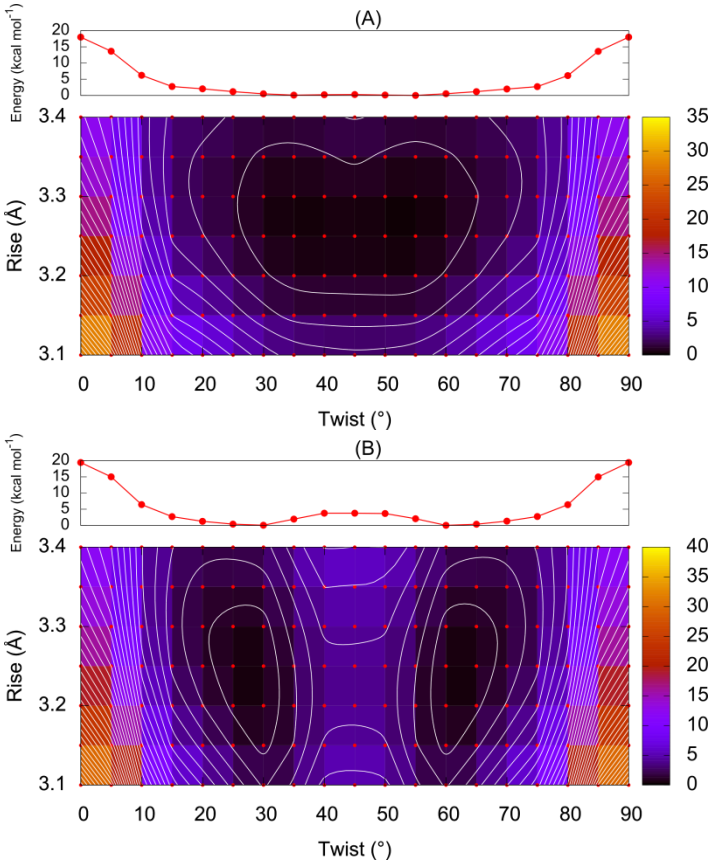
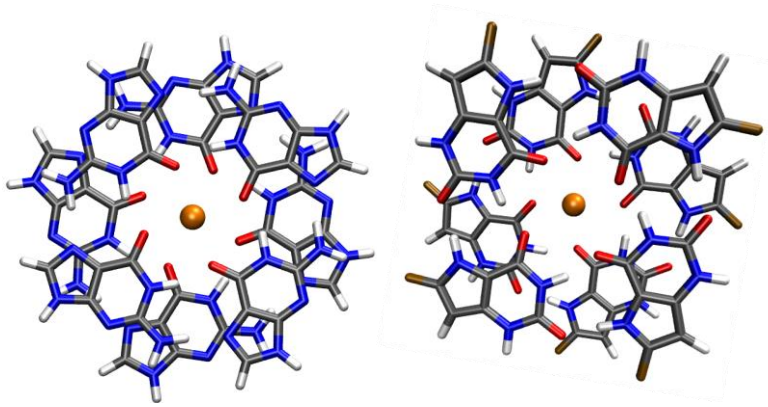


Figure S1. Energy landscapes (color scale in kcal mol^{-1}) resulting from the twist-rise scan of $(G_4)_2 \cdot K^+$ **(A)** and $(FdaX_4)_2 \cdot K^+$ **(B)**. 1D plot represents the horizontal section of energy surface at the constant rise level crossing the local minima (3.25 Å). Equilibrium structures of both models are shown below.



Formation energies for $(B_4)_2 \cdot M^+$ with selected –H and –CH_3 capped derivatives

The structures of $(3\text{-}CH_3X_4)_2 \cdot Na^+$, $(3\text{-}CH_3FdaX_4)_2 \cdot Na^+$, and $(9\text{-}CH_3G_4)_2 \cdot Na^+$ systems and their building blocks were fully optimized by using the BLYP-D3/def2-TZVPP and the energy contributions related to the individual formation steps were calculated at the same level of theory using COSMO model of water.

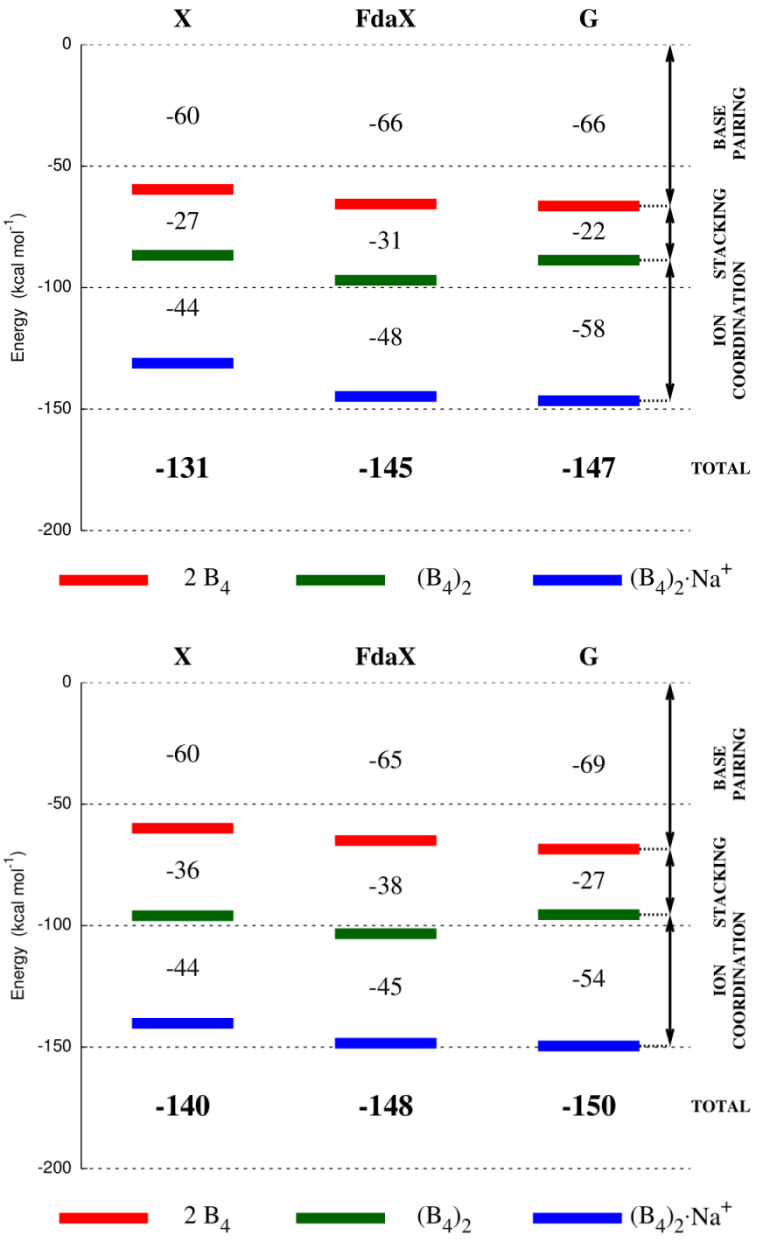


Figure S2. Contributions to the formation energy (ΔE) of the $(B_4)_2 \cdot M^+$ system (in water - COSMO) build from selected derivatives bearing -H atom (top) and -CH_3 group (bottom) at the position of glycosidic bond. Total values of the formation energy are marked in bold. The other three values represent individual contributions of base pairing calculated as $\Delta E = 2 \times \{E[B_4] - 4 \times E[B]\}$, stacking calculated as $\Delta E = E[(B_4)_2] - 2 \times E[B_4]$, and ion coordination calculated as $\Delta E = E[(B_4)_2 \cdot Na^+] - \{E[(B_4)_2] + E[Na^+]\}$.

Comparison of COSMO and SMD implicit models of water environment for $(B_4)_2 \cdot M^+$

The optimized structures of $(B_4)_2 \cdot Na^+$ were subjected to the single-point-energy calculation carried out in Gaussian 09 package[19] employing BLYP-D3/def2-TZVPP level of theory. The effect of water environment was incorporated by the SMD model,[20] which also includes non-polar contribution to solvation energy. The formation energies calculated using COSMO and SMD solvent models are shown in Figure S3.

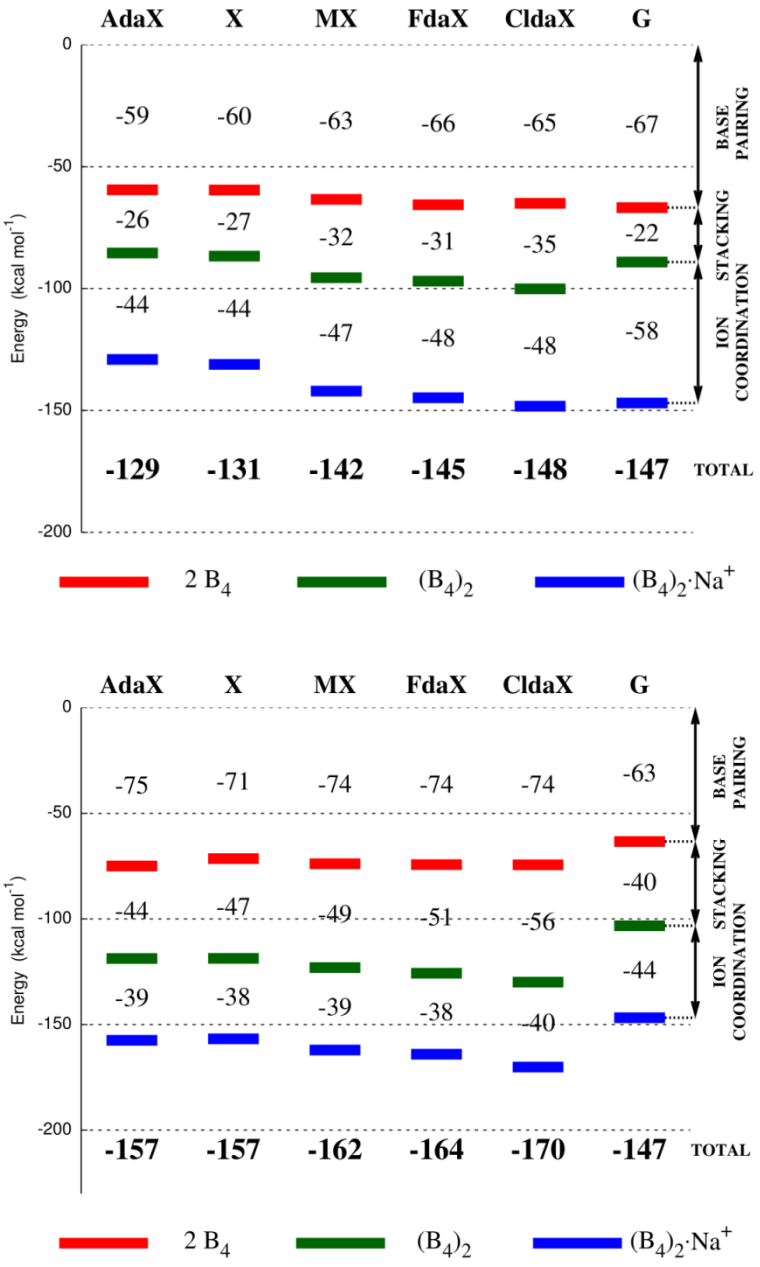


Figure S3. Formation energies calculated in water environment approximated by COSMO (top) and SMD (bottom) solvent models performed on identical DFT structures.

Comparison of MP2 and DFT-D3 for $(B_4)_2 \cdot M^+$

The formation energies of $(B_4)_2 \cdot Na^+$ were also recalculated using RI-MP2/def2-TZVPP in vacuum by using Orca 2.8.[17] The contribution of solvent was omitted in this comparative study. The step termed *base pairing* was obtained as a sum of deformation energies of 8 single bases, formation of four Hoogsteen dimers, and formation of two tetrad whose geometry comes from empty $(B_4)_2$. The step called *stacking* refers to the interaction between two identical tetrads. The last step corresponding to *ion coordination* was calculated as sum of deformation energy (between two-stacked model with and without coordinated Na^+ cation) and interaction energy of Na^+ with adapted two-stacked model. The minor geometrical deviations (e.g., two dimers within the single tetrad or upper and lower tetrad) of equivalent components were neglected. The standard counterpoise correction[18] to interaction energy was applied for every formation step.

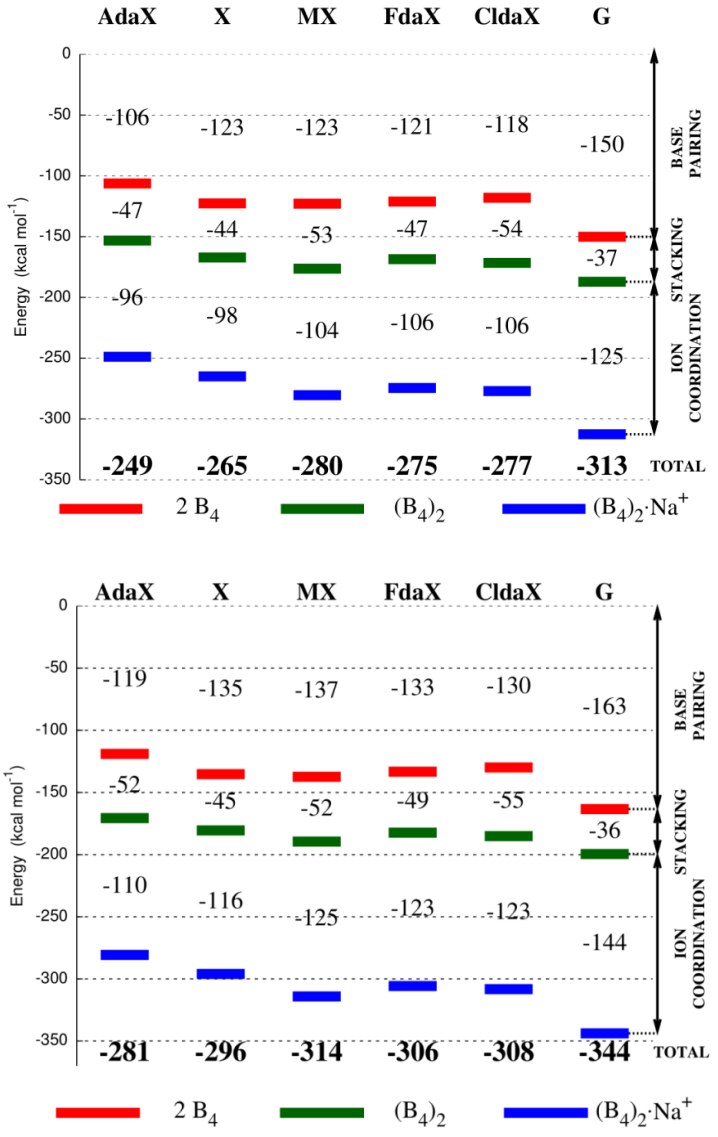


Figure S4. Formation energies calculated at the MP2/def2-TZVPP (top) and BLYP-D3/def2-TZVPP (bottom) levels of theory in vacuum on identical DFT geometries.

Comparison of COSMO and SMD models of implicit water solvent for $(B_4)_3 \cdot 2M^+$

The optimized structures of $(B_4)_3 \cdot 2Na^+$ were subjected to the single point energy calculations analogously to those for $(B_4)_2 \cdot Na^+$.

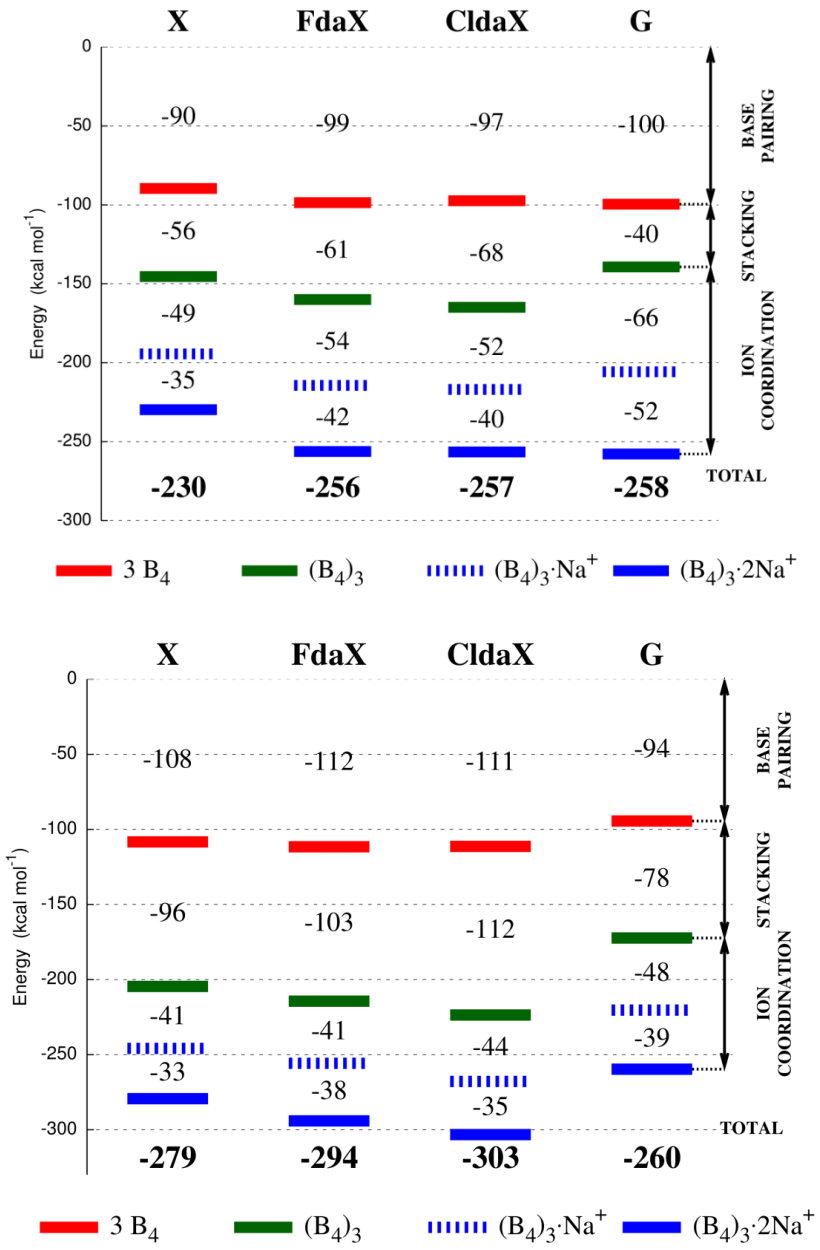


Figure S5. Formation energies for xanthine and guanine $(B_4)_3 \cdot 2Na^+$ systems calculated using COSMO (top) and SMD (bottom) models of water environment performed on identical DFT structures. The other four values represent individual contributions of the base pairing calculated as $\Delta E = 3 \times \{E[B_4] - 4 \times E[B]\}$, the stacking calculated as $\Delta E = E[(B_4)_3] - 3 \times E[B_4]$, the first-ion coordination calculated as $\Delta E = E[(B_4)_3 \cdot Na^+] - \{E[(B_4)_3] + E[Na^+]\}$, and second-ion coordination calculated as $\Delta E = E[(B_4)_3 \cdot 2Na^+] - \{E[(B_4)_3 \cdot Na^+] + E[Na^+]\}$.

Energy barrier to ion transport through the $(B_4)_3$ system

The ion transport was studied at the DFT-D3 level on system composed from three stacked tetrads. The model was prepared from the $(B_4)_3 \cdot 2M^+$ assembly. The planarity of all tetrads were achieved by applying restraints on the torsion angles $(C8\text{-}N1)_i\text{-}(N1\text{-}C8)_j$ between bases *i* and *j* of each opposite base pairs. After that both cations were removed and models containing only one M^+ cation at position with incremented *z* coordinate (from -2 to +2 Å with respect to the central plane) were subjected to partial optimization of central tetrad (positions of all remaining atoms were fixed) using smaller basis set def2-SVP. The final single point energy for each cation position was recalculated employing def2-TZVPP basis set. All calculations including geometry optimization were performed in water environment represented by the COSMO model.

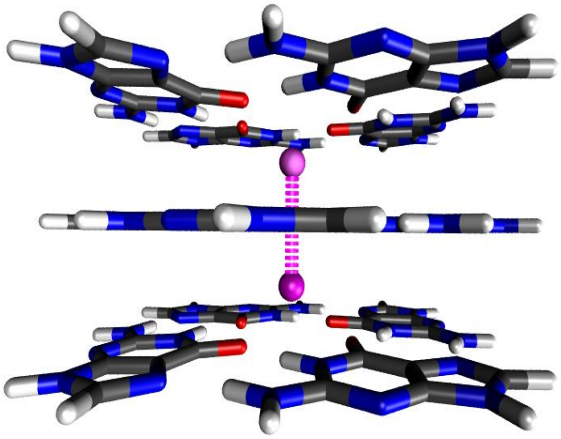


Figure S6. System of three tetrads used in the study of cation transport through the middle tetrad.

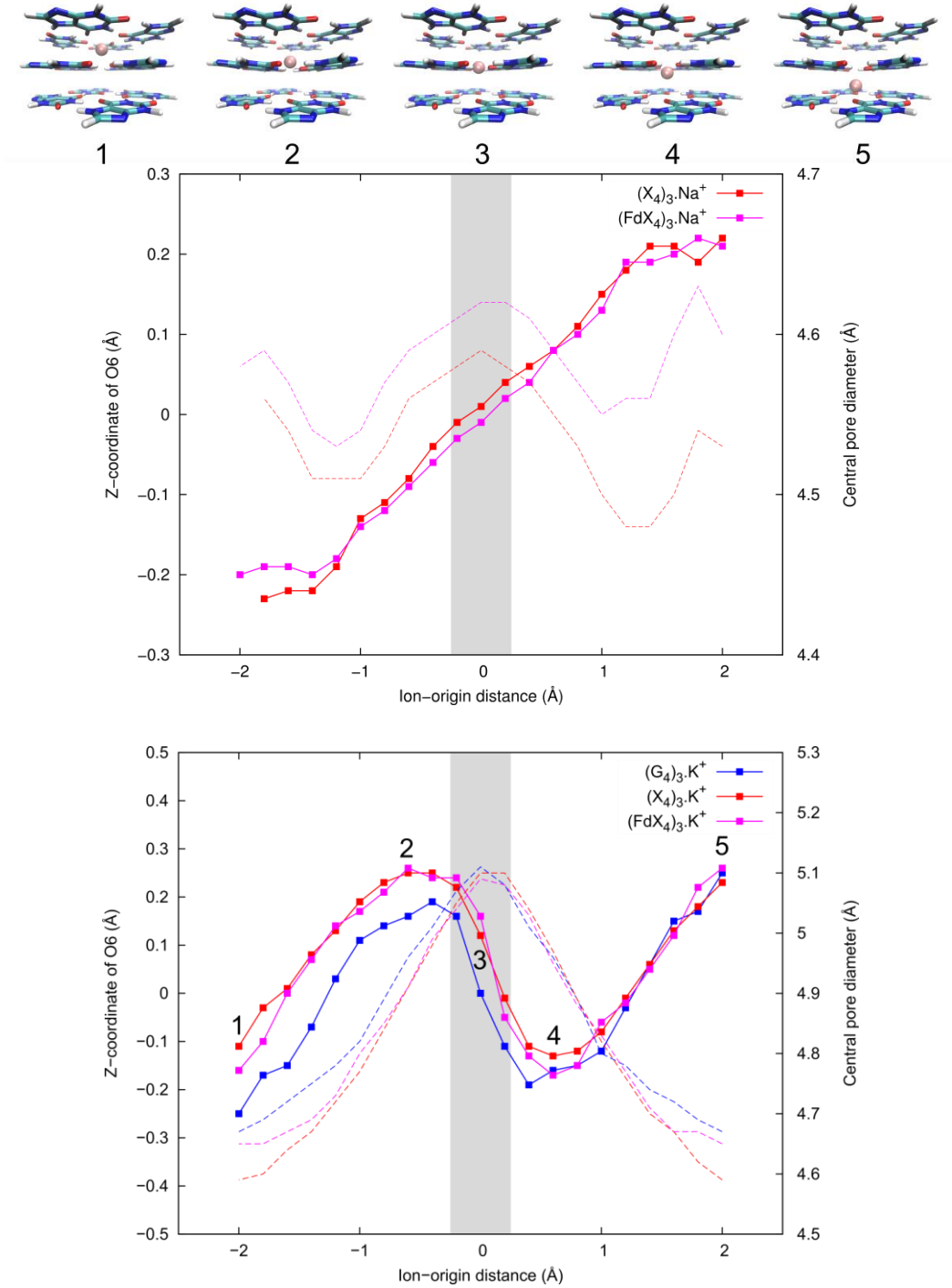


Figure S7. The evolution of the inclination (expressed as averaged *z* coordinate of O6 atoms relative to geometrical center of terminal quartets, depicted by solid lines with squares) and the diameter (dashed lines) of central pore (mean value of distances between opposite O6 atoms) upon penetration of cation through the central tetrad during the potential energy scan.

MD simulations

All structures of xanthine $d(X_4)_4$ or 8F-9deazaxanthine $d(FdaX_4)_4$ based quadruplexes were derived from $d(TG_4T)_4$ structure[2,3] (PDB ID 139D) which was modified and subsequently equilibrated using Avogadro program.[21]

Extra parameterization was performed because none of xanthine building blocks (5´dX, dX and 3´dX residues and corresponding FdaX derivatives) was part of ff99bsc0 force field employed in this study.[22,23] Individual residues were extracted from the $d(X_4)_4$ structure and open valences along the backbone were capped by terminal groups in the same way as described in the work of Cieplak.[24] Structures were then subjected to optimization and electrostatic potential calculation at HF/6-31G* level of theory performed using Gaussian 09 package.[19] The RESP charges[25] (Table S3) were fitted by the antechamber tool[26] in accordance with AMBER[27] force field rules (total charge of 5'-terminal/inner/3'-terminal residue was set to -0.3079/-1.0000/-0.6921, respectively). The atom types and force-field parameters were assigned by parmcheck program. In the case of missing types, parameters suggested by the parmcheck program were used.

Individual models were completed by inserting cations into the quadruplex channel. Models were further solvated by TIP3PBOX water molecules and neutralized using Solvate 1.0 program.[28] The truncated octahedral box with overall minimum distance among replicas of ~12 Å was used. We applied monovalent ion parameters from Joung & Cheatham.[29]

Equilibration of the system and unbiased molecular dynamics simulations were carried out in the sander and pmemd programs of AMBER 11 package.[27] The equilibration protocol included following stages: water and counter ions minimization at constant volume, 2 ps isochoric dynamics of solvent and counter ions, isobaric heating of water and counter ions during 30 ps (with SHAKE), isobaric equilibration of solvent during 100 ps at 298K, cooling of water and counter ions during 30 ps to 0 K, sequence of isochoric minimization (without SHAKE[30]) of water and counter ions with decreasing restraints applied to solute (250, 125, 50, 5, 0 kcal mol^{-1} $Å^{-2}$), 50 fs dynamics at isochoric conditions of the whole system, 2 ps dynamics at 5 K, isobaric heating of the whole system during 50 ps to 150 K (with SHAKE), 5 ps isobaric dynamics of whole system at 150 K, isobaric heating of the whole system during 50 ps to 250 K, 5 ps isobaric dynamics of whole system at 250 K, isobaric heating of the whole system during 50 ps to 298 K, equilibration of the whole system during 50 ps (with SHAKE).

Long-range electrostatic interactions were calculated by using particle-mesh Ewald technique[31] with a 9 Å cutoff for a direct summation. The production simulations were carried out at constant temperature of 298K and constant pressure of 1 bar using 2 fs integration time step and SHAKE. We used Berendsen thermostat employing 1 ps relaxation time and barostat with the relaxation time of 1.2 ps.

Table S4. RESP charges assigned to individual atoms of deoxyribonucleotides employed in MD simulations.

Atom	**G**	**X**	**fdX**	**9fdX**
H1	**0.3520**	**0.3339**	**0.3275**	**0.3127**
N1	-0.5053	-0.4089	-0.4093	-0.3652
C2	0.7432	0.5417	0.5492	0.5366
NH2/O2	**0.4235**	**-0.5613**	**-0.5868**	**-0.5692**
N3	-0.6636	-0.0884	0.0363	-0.2265
C4	0.1814	0.2149	-0.0629	-0.0787
C5	0.1991	-0.0224	-0.0349	0.0323
C6	0.4918	0.4603	0.5086	0.5052
O6	**-0.5699**	**-0.5266**	**-0.5502**	**-0.5516**
N7	-0.5725	-0.2940	-0.3692	-0.4843
H7	**-**	**0.3533**	**0.3833**	**0.4085**
C8	0.0736	0.0560	0.3121	0.3943
H8/F8	0.1997	0.1772	-0.1477	-0.1218
N9/C9-H9	0.0577	-0.3096	-0.2323 0.1798	-0.0883
C1'	0.0358	0.0216	0.0164	-0.0262
H1'	0.1746	0.1586	0.2038	0.1944
C2'	-0.0854	-0.1151	-0.0577	-0.1281
H2', H2''	0.0718	0.0700	0.0665	0.0886
C3'	0.0713	0.3177	0.1560	0.1258
O3'	-0.5232	-0.5232	-0.5232	-0.5232
H3'	0.0985	0.0161	0.0956	0.1098
C4'	0.1629	-0.0334	0.0959	0.0949
H4'	0.1176	0.1221	0.0901	0.0768
O4'	-0.3691	-0.2790	-0.3604	-0.3497
C5'	-0.0069	-0.0748	-0.0853	-0.0167
H5', H5''	0.0754	0.1025	0.1068	0.0805
O5'	-0.4954	-0.4954	-0.4954	-0.4954
P	1.1659	1.1659	1.1659	1.1659
O1P, O2P	-0.7761	-0.7761	-0.7761	-0.7761

ABF simulations

Starting structures were obtained from unbiased MD of model containing single cation in the quadruplex channel. The 10 ns long ABF (Adaptive Biasing Force)[31] simulations were carried out using modified *pmemd* module of AMBER package. To avoid structure corruption, terminal oxygen atoms were fixed by the geometrical restrains with force constant of 10 kcal mol^{-1}. The free energy was calculated along a collective variable (CV), which was defined as an oriented distance of the cation to the plane. The plane was constructed as the best fit plane among heavy atoms of the tetrad bases. Zero value of used CV represents situation for which the ion is located approximately in the plane of the second tetrad. The interval sampled in the range from -2 to +2 Å was discretized into 100 bins. The MD setup was identical to those used in unbiased simulations.

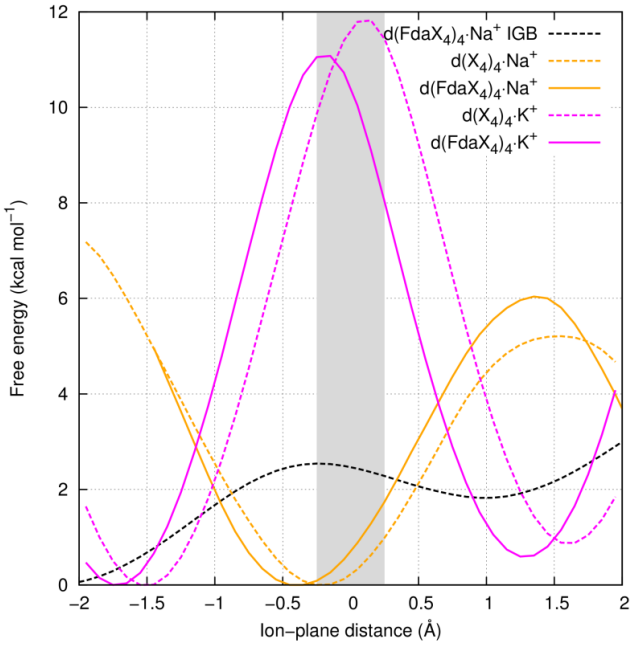


Figure S8. Barrier to ion transport calculated by ABF approach.

Comparison of RMSDs values for unbiased MD simulations

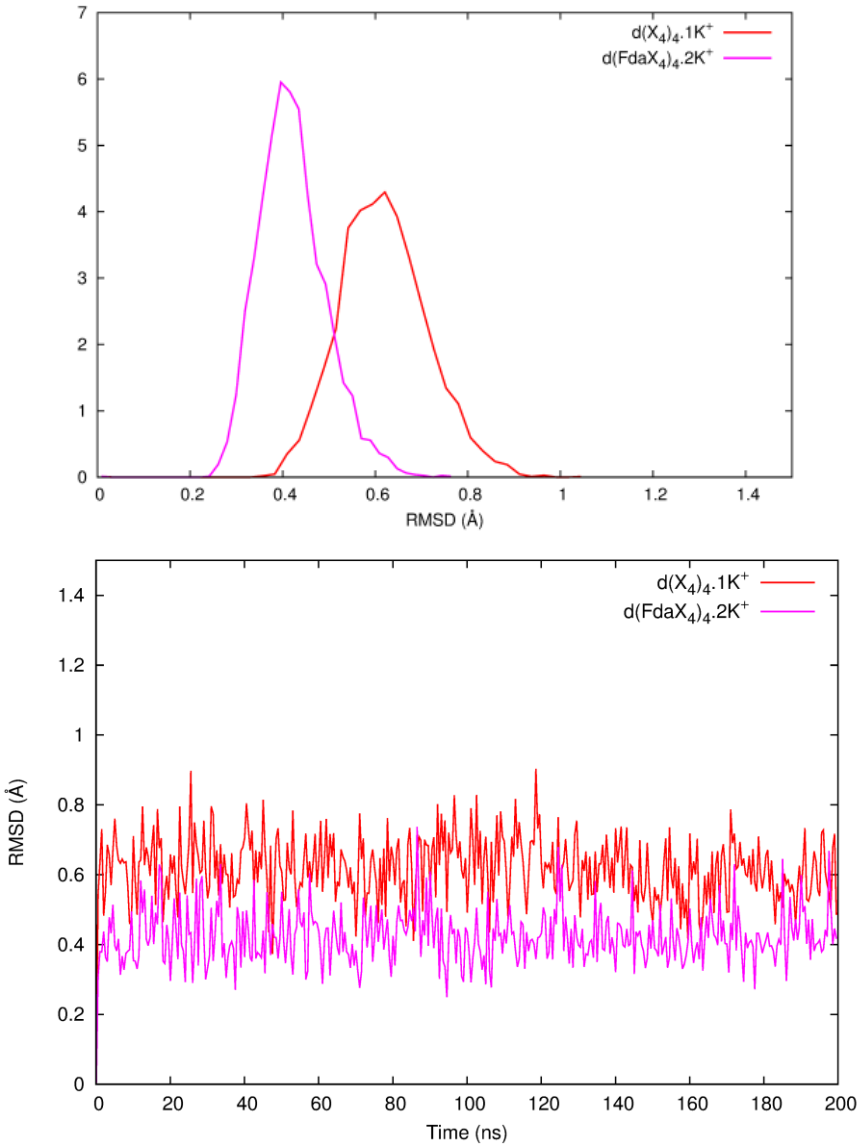


Figure S9. The RMSD distribution (top) and RMSD evolution (bottom) during 200 ns long MD simulation for quadruplex composed of X (red) and 9-FdaX (magenta) bases. The equilibrated structure was used as a reference structure.

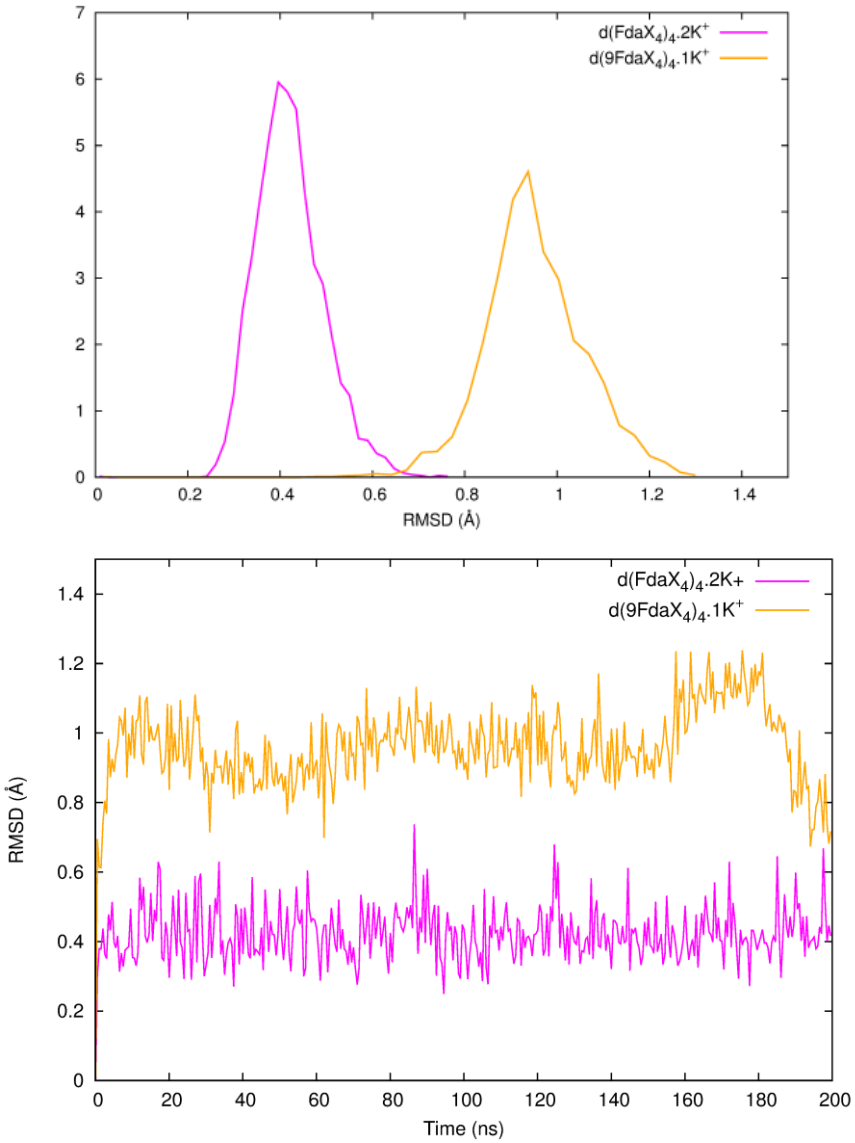


Figure S10. The RMSD distribution (top) and RMSD evolution (bottom) during 200 ns long MD simulation for quadruplexes composed of 3-FdaX (magenta) and 9-FdaX (yellow) bases. The equilibrated structure was used as a reference structure.

Structures of selected $B_{4/8/12}$ models

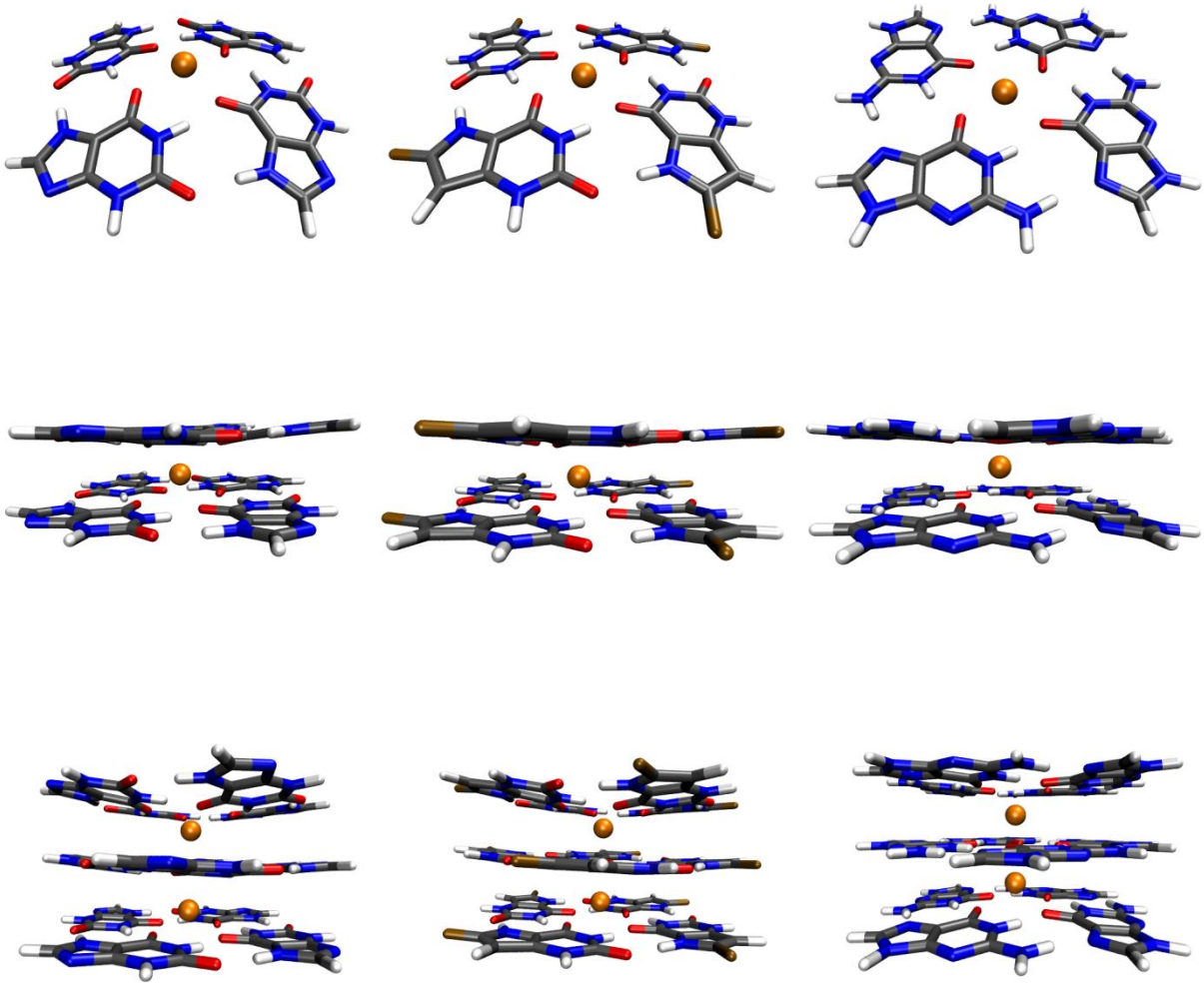


Figure S11. Visualization of optimized $B_4 \cdot Na^+$ (top), $(B_4)_2 \cdot Na^+$ (middle), and $(B_4)_3 \cdot 2Na^+$ systems containing X (left), FdaX (middle), and G (right) unit.

XYZ coordinates of selected $B_{4/8/12}$ models

X4.Na+

N	5.8141238	-1.6937747	-0.5947748
C	5.0937283	-0.8111863	-1.3769066
O	5.2064307	-0.7758311	-2.6161903
N	4.2332088	0.0397371	-0.6887159
H	3.6688720	0.6826270	-1.2719554
C	4.0017389	0.1008642	0.6936711
O	3.1934793	0.9405538	1.1616934
C	4.7655044	-0.8580183	1.4127255
C	5.6505809	-1.7284245	0.7728018
N	6.2702608	-2.5557231	1.6593864
C	5.7560906	-2.1920691	2.8511988
H	6.0194339	-2.6471773	3.7979166
N	4.8548056	-1.1810435	2.7587206
H	4.3075468	-0.7600717	3.5313710
H	6.4533367	-2.3306096	-1.0640289
N	1.3296917	0.6123137	5.8606487
C	2.2110132	0.4901811	4.8031988
O	3.2486226	-0.1932831	4.8773936
N	1.8642251	1.1839520	3.6468599
H	2.5031703	1.0683748	2.8405727
C	0.7302706	1.9792774	3.4238693
O	0.5701497	2.5543645	2.3188398
C	-0.1296852	2.0238760	4.5545149
C	0.1750305	1.3544060	5.7417152
N	-0.7894981	1.5404967	6.6848578
C	-1.6947558	2.3257664	6.0676909
H	-2.6134812	2.6766721	6.5210904
N	-1.3462707	2.6453096	4.7950978
H	-1.8969109	3.2052851	4.1191106
H	1.5514906	0.1196950	6.7223085
N	-3.8882956	4.4709806	0.8624290
C	-2.8554615	4.0706414	1.6887371
O	-2.9718369	4.0301590	2.9274062
N	-1.6722859	3.7166288	1.0458386
H	-0.9051890	3.3862027	1.6576695
C	-1.4077906	3.7052845	-0.3319195
O	-0.2747531	3.3655687	-0.7540972
C	-2.5329012	4.1066800	-1.1018973
C	-3.7396101	4.4818409	-0.5072221
N	-4.6720030	4.8269635	-1.4378112
C	-4.0321282	4.6565087	-2.6119330
H	-4.4752876	4.8341131	-3.5839588
N	-2.7517131	4.2295734	-2.4661051
H	-2.0806874	3.9998821	-3.2215306
H	-4.7678537	4.7378071	1.2977690
N	0.5827702	2.1445736	-5.5963804
C	0.0205295	2.7590290	-4.4935572
O	-1.0200122	3.4380064	-4.5686259
N	0.6952267	2.5714637	-3.2901446
H	0.2606077	3.0019191	-2.4549469
C	1.8634170	1.8291171	-3.0614361
O	2.3576675	1.7694295	-1.9084166
C	2.3526103	1.2125096	-4.2448227
C	1.7204599	1.3764122	-5.4792637
N	2.3658585	0.6976668	-6.4678747
C	3.3983756	0.1090730	-5.8320232
H	4.1327262	-0.5262645	-6.3114885
N	3.4373135	0.3875853	-4.5037786
H	4.1130298	0.0214785	-3.8086433
H	0.1168364	2.2605580	-6.4929175
Na	1.6611579	2.4640414	0.2322603

FdaX4.Na+

N	3.4772094	0.4583537	-4.5290170
N	0.5854353	2.4303148	-3.3053695
N	0.5957308	2.2466778	-5.6396292
N	-2.7570195	4.2786401	-2.4507561
N	-1.7557348	3.5975716	1.0540129
N	-3.8474602	4.6425104	0.9276401
N	5.9542311	-1.5868840	-0.6340554
N	4.1566122	-0.0888098	-0.7192249
N	4.9048071	-1.1622782	2.7501837
N	1.4091370	0.6546336	5.9171997
N	1.7775214	1.0219311	3.6342386
N	-1.2965311	2.7136420	4.8332386
C	2.5498712	0.8992930	-6.5770505
C	-4.6247184	5.1497468	-1.4498020
C	6.5434444	-2.3856949	1.7171471
C	-0.6905897	1.7779881	6.8348074
C	3.5791526	0.2808635	-5.8704973
C	1.7569382	1.4974184	-5.5684114
C	5.1218591	-0.8064816	-1.4102942
C	3.9312244	-0.0706747	0.6661352
C	4.8180744	-0.9078397	1.3836014
C	5.8217681	-1.6566776	0.7416287
C	5.9279775	-2.0378937	2.9177213
C	2.2009817	0.4220152	4.8111602
C	0.6442985	1.8279915	3.4429833
C	-0.1175305	2.0026622	4.6225991
C	0.2610134	1.4240621	5.8483503
C	-1.6122346	2.5621031	6.1443093
C	-2.8596468	4.1022170	1.7256868
C	-1.5345120	3.5718890	-0.3318898
C	-2.6006446	4.1323678	-1.0745348
C	2.3329979	1.2228167	-4.3141112
C	1.7642823	1.6944565	-3.1073321
C	-0.0323557	2.7310733	-4.5103769
C	-3.9588794	4.8786732	-2.6432407
C	-3.7450118	4.6650162	-0.4522603
O	0.4063423	2.3070136	2.3018495
O	3.2308594	-0.2810768	4.8628186
O	3.0098371	0.6481576	1.1375411
O	5.2280238	-0.7474796	-2.6524301
O	-2.9498504	4.0687197	2.9699781
O	-0.4654792	3.0800082	-0.7825670
O	-1.0869900	3.3963007	-4.5660066
O	2.2008839	1.5209481	-1.9379250
H	0.1620305	2.4568849	-6.5339567
H	3.5197324	0.4909356	-1.2954855
H	4.2868459	-0.7909995	3.4967721
H	6.6710493	-2.1190421	-1.1189167
H	2.3558001	0.8357898	2.7948219
H	-1.8525039	3.2291614	4.1245788
H	1.7013817	0.2269581	6.7911670
H	-1.0147939	3.1783823	1.6448732
H	-2.1030914	3.9637439	-3.1926728
H	4.1123634	0.0647732	-3.8086865
H	-4.6644114	5.0207853	1.3984521
H	0.1098286	2.7742313	-2.4514291
F	6.2329362	-2.4635834	4.1508318
F	-2.7181313	3.1455188	6.6253054
F	-4.3709340	5.1383540	-3.8912852
F	4.6002054	-0.4331814	-6.3627534
Na	1.3767825	2.0247309	0.1924414
H	-5.5903251	5.6217961	-1.3370905
H	2.4100313	0.9064400	-7.6486441
H	7.3782591	-3.0593623	1.5860935
H	-0.7174012	1.5143684	7.8825318

G4.Na+

N	-3.4323003	-4.4369084	1.5607643
O	0.6520234	-2.2189749	1.5878845
N	-1.3404843	-3.3905901	1.5699992
C	-2.0908686	-4.5602897	1.5508672
N	-1.5334473	-5.7796672	1.5271660
C	-0.1857306	-5.7524391	1.5265100
C	0.6574581	-4.6258591	1.5465530
C	0.0647802	-3.3350093	1.5695530
N	0.6697354	-6.8337095	1.5059427
C	1.9616510	-6.3387610	1.5138091
N	1.9938389	-5.0171225	1.5383795
H	-3.9330692	-3.5300639	1.5733770
H	-3.9756179	-5.2914055	1.5436760
H	-1.8240612	-2.4742477	1.5842527
H	0.4022462	-7.8128574	1.4868084
H	2.8232598	-6.9945671	1.5010246
N	-4.4355070	3.4312190	1.6277946
O	-2.2191826	-0.6542681	1.6088272
N	-3.3897990	1.3390640	1.6138332
C	-4.5594272	2.0898173	1.6173538
N	-5.7792616	1.5329609	1.6132294
C	-5.7526589	0.1852502	1.6057002
C	-4.6262446	-0.6583641	1.6024687
C	-3.3349330	-0.0662329	1.6078779
N	-6.8344589	-0.6696743	1.5998002
C	-6.3399643	-1.9618086	1.5926084
N	-5.0181220	-1.9945963	1.5941445
H	-3.5288401	3.9318009	1.6041240
H	-5.2901753	3.9744090	1.6152793
H	-2.4733431	1.8224500	1.6164753
H	-7.8136683	-0.4017378	1.5994137
H	-6.9962861	-2.8231056	1.5867389
N	3.4326209	4.4373006	1.5288003
O	-0.6508282	2.2189682	1.6084733
N	1.3411111	3.3909560	1.5666116
C	2.0911547	4.5605413	1.5342655
N	1.5334140	5.7797626	1.5101774
C	0.1857642	5.7523266	1.5214206
C	-0.6571528	4.6258058	1.5546034
C	-0.0641519	3.3351111	1.5791837
N	-0.6698475	6.8334596	1.5024049
C	-1.9616440	6.3385320	1.5237576
N	-1.9935489	5.0170660	1.5560441
H	3.9336161	3.5308093	1.5496838
H	3.9756853	5.2917786	1.5048589
H	1.8249053	2.4747173	1.5792587
H	-0.4025610	7.8124970	1.4762417
H	-2.8234134	6.9941838	1.5140842
N	4.4359289	-3.4307163	1.6221168
O	2.2198400	0.6550048	1.5897476
N	3.3903196	-1.3385354	1.6005729
C	4.5599442	-2.0893141	1.6106085
N	5.7797786	-1.5324746	1.6135381
C	5.7532213	-0.1847520	1.6067941
C	4.6268201	0.6588107	1.5970103
C	3.3355086	0.0667530	1.5948295
N	6.8349751	0.6702714	1.6076861
C	6.3404167	1.9623834	1.5978991
N	5.0185916	1.9950618	1.5918358
H	3.5295121	-3.9313689	1.5929187
H	5.2905922	-3.9740175	1.6156224
H	2.4739355	-1.8221165	1.5985474
H	7.8141805	0.4023687	1.6134060
H	6.9966926	2.8237316	1.5955663
Na	0.0010768	0.0003824	1.5921655

X8.Na+

N	5.1076125	-2.6068524	-3.6032566
C	4.6296296	-1.3085282	-3.6322582
O	5.3846244	-0.3200091	-3.5833344
N	3.2483698	-1.1787933	-3.7062865
H	2.8729311	-0.2096264	-3.7075692
C	2.2805452	-2.1942842	-3.6768794
O	1.0637466	-1.8969978	-3.6510965
C	2.8606339	-3.4913806	-3.6564049
C	4.2430102	-3.6815185	-3.6008366
N	4.5639253	-5.0025953	-3.5235233
C	3.3688426	-5.6267002	-3.5385243
H	3.2369598	-6.7001664	-3.4934351
N	2.3202586	-4.7684996	-3.6202484
H	1.3132415	-5.0092899	-3.6357824
H	6.1135339	-2.7405512	-3.5405065
N	5.7602432	0.2271579	-0.3058568
C	4.7160406	1.1263644	-0.4284531
O	4.8946221	2.3579947	-0.4126357
N	3.4526453	0.5658118	-0.5773466
H	2.6524288	1.2258539	-0.6494495
C	3.1053934	-0.7942592	-0.5883446
O	1.9156256	-1.1354185	-0.7649493
C	4.2367001	-1.6409901	-0.4162870
C	5.5322936	-1.1317978	-0.3140670
N	6.4568129	-2.1307855	-0.2376872
C	5.7206502	-3.2589726	-0.2869715
H	6.1283434	-4.2609967	-0.2448615
N	4.3872955	-3.0207581	-0.3978415
H	3.6248376	-3.7226312	-0.4361576
H	6.7013351	0.6016153	-0.2183434
N	-2.7366742	-5.1561838	-3.5471460
C	-1.4394625	-4.6778776	-3.6065199
O	-0.4498907	-5.4325921	-3.5809007
N	-1.3118604	-3.2965636	-3.6834161
H	-0.3430434	-2.9210142	-3.7071718
C	-2.3265493	-2.3289508	-3.6295927
O	-2.0289405	-1.1121075	-3.6106107
C	-3.6226716	-2.9093721	-3.5783835
C	-3.8111588	-4.2918058	-3.5189116
N	-5.1299926	-4.6130223	-3.4105865
C	-5.7544975	-3.4180531	-3.4102797
H	-6.8266183	-3.2863854	-3.3397380
N	-4.8986718	-2.3692776	-3.5118258
H	-5.1398533	-1.3622910	-3.5205633
H	-2.8686263	-6.1621408	-3.4814426
N	0.1751539	-5.8127616	-0.3189587
C	1.0710694	-4.7683692	-0.4623901
O	2.3027252	-4.9467834	-0.4759974
N	0.5069562	-3.5049350	-0.5969139
H	1.1650298	-2.7045856	-0.6839048
C	-0.8530190	-3.1579576	-0.5758064
O	-1.1985514	-1.9683013	-0.7446196
C	-1.6952837	-4.2894517	-0.3841426
C	-1.1836212	-5.5850158	-0.2947433
N	-2.1803618	-6.5097837	-0.1955856
C	-3.3095315	-5.7738074	-0.2179548
H	-4.3102184	-6.1817363	-0.1526468
N	-3.0742200	-4.4403389	-0.3334961
H	-3.7770094	-3.6780445	-0.3549552
H	0.5516939	-6.7538601	-0.2410407
N	-5.2845984	2.6874207	-3.4228212
C	-4.8076441	1.3903957	-3.4953432
O	-5.5615611	0.4006997	-3.4551316
N	-3.4283680	1.2631148	-3.6029234
H	-3.0533815	0.2943396	-3.6374745
C	-2.4598949	2.2777620	-3.5687879
O	-1.2428926	1.9800122	-3.5775794
C	-3.0390683	3.5737714	-3.5026337
C	-4.4198992	3.7619272	-3.4120730
N	-4.7388408	5.0804955	-3.2944476
C	-3.5442730	5.7052493	-3.3198518
H	-3.4112537	6.7772899	-3.2506283
N	-2.4978796	4.8498070	-3.4461687

H	-1.4914229	5.0913749	-3.4773564
H	-6.2888675	2.8191558	-3.3346206
N	-5.8650373	-0.2298365	-0.1847914
C	-4.8240408	-1.1252084	-0.3540926
O	-5.0025769	-2.3568431	-0.3666296
N	-3.5640605	-0.5605386	-0.5160303
H	-2.7658860	-1.2182041	-0.6237225
C	-3.2169270	0.7994684	-0.4995258
O	-2.0315494	1.1457543	-0.6946632
C	-4.3439170	1.6410346	-0.2802131
C	-5.6370481	1.1289472	-0.1627821
N	-6.5594874	2.1253140	-0.0407177
C	-5.8243580	3.2546662	-0.0772311
H	-6.2308482	4.2551429	-0.0006602
N	-4.4937893	3.0198345	-0.2232542
H	-3.7322470	3.7227277	-0.2605962
H	-6.8040819	-0.6067654	-0.0866413
N	2.5593923	5.2366943	-3.4737816
C	1.2609767	4.7598852	-3.5164877
O	0.2725497	5.5136886	-3.4512916
N	1.1311174	3.3807932	-3.6236392
H	0.1618223	3.0057771	-3.6360505
C	2.1462603	2.4122819	-3.6155024
O	1.8484747	1.1952926	-3.6192629
C	3.4434709	2.9913673	-3.5790378
C	3.6338043	4.3719918	-3.4903294
N	4.9548595	4.6906756	-3.4036036
C	5.5787404	3.4961847	-3.4461933
H	6.6521680	3.3631700	-3.4028815
N	4.7204468	2.4500100	-3.5541317
H	4.9609593	1.4435202	-3.5925165
H	2.6932443	6.2408151	-3.3870844
N	-0.2800164	5.8109427	-0.1680545
C	-1.1791802	4.7702080	-0.3178773
O	-2.4107633	4.9487325	-0.3011642
N	-0.6185365	3.5104557	-0.4949556
H	-1.2786735	2.7124669	-0.5880975
C	0.7414442	3.1632521	-0.5110056
O	1.0829841	1.9780316	-0.7153870
C	1.5879861	4.2899438	-0.3101870
C	1.0788876	5.5828872	-0.1785115
N	2.0779505	6.5050641	-0.0782890
C	3.2060554	5.7699737	-0.1427110
H	4.2080647	6.1764101	-0.0890975
N	2.9677401	4.4396456	-0.2854811
H	3.6694024	3.6780563	-0.3410155
H	-0.6544627	6.7498352	-0.0594534
Na	-0.0751602	0.0270114	-2.3982997

FdaX8.Na+

N	3.4738839	-4.3578663	2.2818030
C	3.0409875	-4.0408805	1.0097763
O	3.6854067	-4.3645302	-0.0090199
N	1.8562401	-3.3286114	0.9387222
H	1.5244361	-3.0668866	-0.0122563
C	1.0713338	-2.8609433	2.0051554
O	0.0556066	-2.1600295	1.7627327
C	1.5731102	-3.2489624	3.2710907
C	2.7714823	-3.9736918	3.4105348
C	3.0487893	-4.1407650	4.7882023
C	1.9841657	-3.5043086	5.4229908
F	1.7710381	-3.3721089	6.7382932
N	1.0944750	-2.9726985	4.5490650
H	0.2171695	-2.4725830	4.7956028
H	4.3460106	-4.8726546	2.3541690
H	3.8868472	-4.6329123	5.2601547
N	5.7875487	-1.7680638	-0.4422143
C	4.8426029	-1.1994263	-1.2722140
O	4.9925163	-1.1537222	-2.5101320
N	3.7143036	-0.6969752	-0.6444471
H	2.9897831	-0.2644879	-1.2527747
C	3.4605128	-0.6308605	0.7370267
O	2.3825572	-0.1368672	1.1447646
C	4.5073292	-1.1879200	1.5166189
C	5.6440261	-1.7752362	0.9337860
C	6.4622418	-2.3072307	1.9606835
C	5.7710816	-2.0025696	3.1315902
F	6.1200873	-2.2901383	4.3929451
N	4.6092532	-1.3415293	2.8974579
H	3.9381270	-1.0061739	3.6177520
H	6.6207948	-2.1435814	-0.8845636
H	7.4051699	-2.8289510	1.8794849
N	-3.1288698	-0.3365449	5.1507818
C	-2.0740610	-1.0452707	4.6119850
O	-1.2402805	-1.6383169	5.3271302
N	-1.9926730	-1.0428287	3.2302917
H	-1.1860426	-1.5456888	2.8091442
C	-2.8271946	-0.3701978	2.3216026
O	-2.5641340	-0.4143479	1.0930644
C	-3.8908663	0.3164410	2.9562065
C	-4.0306708	0.3497669	4.3562145
C	-5.1326696	1.1735145	4.6874583
C	-5.6152481	1.5990004	3.4514660
F	-6.6543155	2.4080692	3.2085806
N	-4.9022762	1.1023909	2.4108728
H	-5.0885207	1.2728095	1.4022944
H	-3.2010329	-0.3210924	6.1633933
H	-5.5212472	1.4333087	5.6615307
N	1.1520553	0.6730554	5.9267184
C	1.8382051	0.2141775	4.8202785
O	2.8955818	-0.4404798	4.9224883
N	1.2699697	0.5144759	3.5930220
H	1.7762042	0.1843900	2.7466582
C	0.1241737	1.2906963	3.3463816
O	-0.2616809	1.4662488	2.1659049
C	-0.4825306	1.7710689	4.5354999
C	0.0086952	1.4435546	5.8115512
C	-0.8489539	2.0039102	6.7899675
C	-1.8260252	2.6594144	6.0434416
F	-2.8794154	3.3540907	6.4943414
N	-1.6347386	2.5353621	4.7056452
H	-2.2270001	2.9524104	3.9590741
H	1.5524643	0.4616565	6.8355797
H	-0.7809988	1.9503366	7.8671881
N	-5.2171078	1.7408508	-2.5536491
C	-4.8600914	1.2988173	-1.2954747
O	-5.4850201	1.6442125	-0.2712374
N	-3.7592584	0.4617016	-1.2422796
H	-3.4492484	0.1568584	-0.2983992
C	-2.9425218	0.0481295	-2.3096661
O	-1.9402290	-0.6712120	-2.0772219
C	-3.3820658	0.5435768	-3.5620421
C	-4.4961589	1.3934607	-3.6832974

C	-4.6376599	1.7725958	-5.0397710
C	-3.5871261	1.1191095	-5.6808606
F	-3.2666955	1.1553669	-6.9808581
N	-2.8340916	0.3785252	-4.8308776
H	-1.9967719	-0.1834125	-5.0807253
H	-6.0191182	2.3607312	-2.6106291
H	-5.3724998	2.4219547	-5.4932495
N	-3.9705973	4.4954965	0.7226174
C	-3.1477261	3.7432858	1.5362320
O	-3.2623446	3.7489457	2.7788482
N	-2.1989770	2.9724457	0.8844318
H	-1.5570808	2.4147738	1.4823335
C	-1.9321886	2.9265402	-0.4952342
O	-1.0339387	2.1650008	-0.9274117
C	-2.7822569	3.7770622	-1.2486055
C	-3.8075391	4.5310599	-0.6506838
C	-4.5260083	5.2120042	-1.6639945
C	-3.8824476	4.8360150	-2.8412965
F	-4.1754047	5.2073452	-4.0950706
N	-2.8480452	3.9849739	-2.6244732
H	-2.2187645	3.5860715	-3.3507270
H	-4.6741385	5.0656033	1.1820035
H	-5.3751352	5.8738567	-1.5700559
N	1.3944070	-2.2737436	-5.4225329
C	0.2588993	-1.6935340	-4.8930066
O	-0.5621793	-1.0776303	-5.6038623
N	0.0982036	-1.8262488	-3.5248618
H	-0.7372835	-1.3692258	-3.1062620
C	0.9721354	-2.4439582	-2.6137914
O	0.7018992	-2.4221336	-1.3872169
C	2.1034301	-3.0212790	-3.2415176
C	2.3222304	-2.9243550	-4.6277211
C	3.5620210	-3.5320194	-4.9398747
C	4.0359660	-3.9768704	-3.7075074
F	5.1843247	-4.6158575	-3.4495476
N	3.1890508	-3.6940743	-2.6872994
H	3.3335475	-3.9305837	-1.6860156
H	1.5332519	-2.1785512	-6.4237330
H	4.0511331	-3.6300705	-5.8982333
N	0.6570392	2.0560956	-5.6365953
C	-0.1517974	2.3227753	-4.5508940
O	-1.1806935	3.0220723	-4.6497633
N	0.2442112	1.7549071	-3.3506475
H	-0.3454435	1.9564265	-2.5184619
C	1.4070038	1.0046522	-3.0999633
O	1.6199424	0.5584702	-1.9476634
C	2.2067458	0.8261623	-4.2588507
C	1.8229984	1.3213491	-5.5176030
C	2.7815544	0.9187790	-6.4799625
C	3.7156286	0.1960905	-5.7404929
F	4.8286524	-0.4057669	-6.1818088
N	3.3987073	0.1242643	-4.4230031
H	3.9517570	-0.3556054	-3.6842717
H	0.3810259	2.4612039	-6.5257958
H	2.8050593	1.1157493	-7.5422825
Na	-0.2199918	-0.3204520	0.0338304

G8.Na+

N	-0.5019224	-1.4947902	6.8568815
C	-1.4897698	-0.5556063	6.6135806
H	-2.0073019	-0.0492894	7.4182607
N	-1.6958012	-0.3719031	5.3212682
C	-0.8012354	-1.2263013	4.6848254
C	-0.5341957	-1.4277864	3.3004183
O	-1.0869381	-0.8694001	2.3217122
N	0.4904981	-2.3738582	3.0935811
H	0.7332416	-2.5433500	2.0970144
C	1.1671598	-3.0449137	4.1012887
N	2.1130527	-3.9336665	3.7334022
H	2.4189342	-4.0846680	2.7538693
H	2.6567232	-4.3521077	4.4776150
N	0.9166051	-2.8533671	5.4040397
C	-0.0466752	-1.9401219	5.6315251
H	-0.1821055	-1.8066870	7.7681105
N	5.1144899	-2.0884108	4.3391944
C	4.2169528	-1.3895850	5.1281300
H	4.2594516	-1.4235088	6.2092058
N	3.3405443	-0.7129495	4.4070343
C	3.6734941	-0.9805364	3.0830357
C	3.0570340	-0.5702123	1.8673912
O	2.0505532	0.1692541	1.7269613
N	3.7064304	-1.1062712	0.7384824
H	3.2794875	-0.8474524	-0.1726325
C	4.8184412	-1.9352037	0.7804888
N	5.3295549	-2.3515827	-0.3957315
H	4.8912739	-2.1567836	-1.3160442
H	6.0829885	-3.0260184	-0.3509967
N	5.3973396	-2.3235780	1.9249593
C	4.7854373	-1.8387579	3.0217146
H	5.8805179	-2.6662670	4.6696754
N	-6.2212428	3.2319788	0.6452023
C	-6.0154952	3.1011983	-0.7178165
H	-6.6200029	3.6341826	-1.4404590
N	-5.0206666	2.2767808	-0.9951917
C	-4.5477711	1.8479248	0.2408482
C	-3.4597454	0.9908117	0.5725079
O	-2.6790098	0.4007989	-0.2132532
N	-3.3053680	0.8501660	1.9668205
H	-2.5100836	0.2476989	2.2591351
C	-4.1086827	1.4584475	2.9199723
N	-3.8375059	1.2069840	4.2173272
H	-3.0208014	0.6572959	4.5442589
H	-4.3749930	1.7238846	4.9017676
N	-5.1313341	2.2665420	2.6071468
C	-5.2902629	2.4338152	1.2803290
H	-6.9338519	3.7993685	1.0926233
N	-2.1566643	4.2073024	5.1835704
C	-2.8227588	4.6393576	4.0496503
H	-3.6567618	5.3272370	4.1038816
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C	-1.2812126	3.2939352	3.3719687
C	-0.4113604	2.4372329	2.6399308
O	-0.3861861	2.2455000	1.3979991
N	0.4893004	1.7554606	3.4810721
H	1.1359997	1.1065572	2.9909177
C	0.5424350	1.8865623	4.8614514
N	1.4748398	1.1689584	5.5198395
H	2.0951338	0.4726337	5.0646525
H	1.4491909	1.2080854	6.5308923
N	-0.2787195	2.6903652	5.5510247
C	-1.1610554	3.3437197	4.7720355
H	-2.3558438	4.4853882	6.1390480
N	-1.6457270	-0.9842094	-6.7684250
C	-0.5611020	-1.8108634	-6.5291708
H	-0.0092815	-2.2770539	-7.3353122
N	-0.3059902	-1.9380605	-5.2388061
C	-1.2635849	-1.1571670	-4.5996610
C	-1.4567038	-0.8699747	-3.2182157
O	-0.7890429	-1.2955282	-2.2441258
N	-2.5383796	0.0094995	-3.0087059
H	-2.7079859	0.2639329	-2.0149637

C	-3.3361481	0.5400997	-4.0115354
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H	-4.8628966	1.8039696	-4.3863078
N	-3.1530242	0.2705901	-5.3116839
C	-2.1136503	-0.5540312	-5.5424406
H	-2.0316878	-0.7486331	-7.6769693
N	-2.9665324	4.5648704	-4.4271320
C	-2.1714098	3.7470051	-5.2113694
H	-2.2476253	3.7410599	-6.2910992
N	-1.3503205	3.0069131	-4.4875632
C	-1.6184291	3.3501787	-3.1662859
C	-1.0819727	2.8486090	-1.9469375
O	-0.2000766	1.9648338	-1.8003158
N	-1.6676516	3.4593984	-0.8212962
H	-1.3163994	3.1132707	0.0932318
C	-2.6508938	4.4374857	-0.8692471
N	-3.0971034	4.9299250	0.3038026
H	-2.8072356	4.5637524	1.2306427
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N	-3.1585445	4.9072566	-2.0170248
C	-2.6270564	4.3282753	-3.1099225
H	-3.6603732	5.2259106	-4.7611370
N	4.0866288	-5.6949354	-0.5568785
C	3.9762265	-5.4529112	0.8019755
H	4.6175550	-5.9427140	1.5234070
N	3.0258677	-4.5768469	1.0769240
C	2.4884147	-4.2235435	-0.1566333
C	1.4695305	-3.2865688	-0.4916438
O	0.7998775	-2.5675332	0.2892969
N	1.2574798	-3.2136582	-1.8835614
H	0.5331866	-2.5290000	-2.1793367
C	1.9428502	-3.9590328	-2.8314155
N	1.6089228	-3.7807962	-4.1262516
H	0.9340348	-3.0668491	-4.4591429
H	2.1727365	-4.2674100	-4.8116818
N	2.9026002	-4.8397843	-2.5154560
C	3.1387731	-4.9167312	-1.1918471
H	4.7354417	-6.3364185	-1.0012424
N	4.3075877	-1.7227287	-5.2727487
C	4.8725996	-2.2725634	-4.1348797
H	5.6753245	-2.9967611	-4.1882056
N	4.3146958	-1.8128762	-3.0288551
C	3.3355283	-0.9222126	-3.4571201
C	2.3838015	-0.1612482	-2.7214425
O	2.2342631	-0.1154010	-1.4742519
N	1.5447681	0.5926867	-3.5648148
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C	1.6195766	0.6109074	-4.9504379
N	0.7473241	1.3983713	-5.6108911
H	-0.0168366	1.9277255	-5.1496096
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Na	0.0999560	0.1149506	-0.0109857

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N	-0.0956748	-6.0931187	4.4344522
C	0.0985220	-6.1557578	3.0662886
O	1.0848751	-6.7170976	2.5568344
N	-0.8673345	-5.5209065	2.2940393
H	-0.7271592	-5.5483439	1.2650963
C	-1.9817906	-4.7910362	2.7292549
O	-2.7073148	-4.2030276	1.8908890
C	-2.1154899	-4.7991320	4.1426134
C	-1.1795997	-5.4287756	4.9679338
N	-1.4758175	-5.2540343	6.2846626
C	-2.6072868	-4.5209913	6.2675338
H	-3.1405414	-4.1951156	7.1514491
N	-3.0309701	-4.2236375	5.0122750
H	-3.8738131	-3.6837048	4.7474622
H	0.5904451	-6.5476204	5.0318658
N	3.3214363	-4.2980994	2.5260713
C	2.9217721	-4.0440361	1.2266157
O	3.6153670	-4.3574186	0.2439557
N	1.6942538	-3.4054143	1.0878416
H	1.3881070	-3.1807961	0.1195965
C	0.8585389	-2.9092844	2.0986087
O	-0.1968622	-2.3070234	1.7931788
C	1.3600023	-3.1905016	3.3981144
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N	0.8769452	-2.9396390	4.6758009
H	0.0109804	-2.4234128	4.9160281
H	4.2086303	-4.7752277	2.6642523
N	5.7362297	-1.7872153	0.0885844
C	4.8475795	-1.3094838	-0.8552397
O	5.0875282	-1.3416861	-2.0747751
N	3.6494743	-0.8069087	-0.3538333
H	2.9836930	-0.4146264	-1.0467214
C	3.2654033	-0.6699470	0.9864576
O	2.1284175	-0.2182447	1.2683099
C	4.2637937	-1.1292140	1.8864541
C	5.4566817	-1.7015674	1.4336938
N	6.2251777	-2.1396355	2.4688432
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N	4.3239713	-1.2215282	3.2705755
H	3.6189600	-0.8709187	3.9460969
H	6.6189305	-2.1703123	-0.2407513
N	-6.8083551	-1.5319245	2.9568541
C	-5.7037137	-2.3423476	3.1484306
O	-5.3051639	-2.6709129	4.2801260
N	-5.0452415	-2.7420100	1.9912861
H	-4.2071057	-3.3419405	2.1201458
C	-5.3341897	-2.3906782	0.6656218
O	-4.5768453	-2.7726205	-0.2592614
C	-6.4941699	-1.5788489	0.5615799
C	-7.2011851	-1.1548302	1.6902718
N	-8.2385048	-0.3404903	1.3541244
C	-8.1743301	-0.2727262	0.0091059
H	-8.8600371	0.2914721	-0.6100336
N	-7.1502614	-0.9953603	-0.5129690
H	-6.9061627	-1.1026179	-1.5134195
H	-7.3185426	-1.2241956	3.7810086
N	-3.3120368	-0.1574659	5.0588959
C	-2.2733116	-0.9341757	4.5786000
O	-1.4563471	-1.4919705	5.3310348
N	-2.1939555	-1.0446696	3.1945876
H	-1.4044445	-1.6039459	2.8130446
C	-2.9772774	-0.3964652	2.2287481
O	-2.7325943	-0.5680677	1.0119140
C	-4.0004302	0.3992458	2.8113346
C	-4.1662962	0.4941995	4.1967123
N	-5.2219011	1.2901184	4.5199381
C	-5.7094139	1.6865098	3.3272709
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N	-5.0188681	1.1763126	2.2749019

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N	0.6780910	0.9967484	5.9323820
C	1.4109122	0.4120868	4.9175034
O	2.4275763	-0.2695320	5.1354917
N	0.9240224	0.6166530	3.6288690
H	1.4820583	0.2133949	2.8521856
C	-0.1761599	1.3895684	3.2351615
O	-0.4985132	1.4471875	2.0229278
C	-0.8313734	2.0014900	4.3368625
C	-0.4214538	1.7769137	5.6549046
N	-1.2415226	2.3990911	6.5461664
C	-2.1531001	3.0193020	5.7708663
H	-2.9675273	3.6262358	6.1455458
N	-1.9549138	2.8104372	4.4432857
H	-2.5134516	3.2015210	3.6613409
H	0.9978520	0.8612974	6.8883049
N	-5.2249228	-1.8222472	-5.1337246
C	-5.4754538	-1.8441675	-3.7733688
O	-6.4249452	-1.2262290	-3.2594250
N	-4.5753185	-2.5781575	-3.0095866
H	-4.7446228	-2.5953077	-1.9847852
C	-3.4280210	-3.2585532	-3.4398239
O	-2.6723455	-3.8006151	-2.5973060
C	-3.2629432	-3.2034602	-4.8487471
C	-4.1418813	-2.4882604	-5.6669931
N	-3.7556096	-2.5282324	-6.9713785
C	-2.6380296	-3.2822900	-6.9551849
H	-2.0552979	-3.5342563	-7.8320007
N	-2.3018378	-3.7106963	-5.7114715
H	-1.4948405	-4.3047726	-5.4507673
H	-5.8662769	-1.2996224	-5.7251145
N	-5.0994987	1.7499671	-2.7342696
C	-4.8235869	1.3102787	-1.4522549
O	-5.4713955	1.6939110	-0.4633133
N	-3.7652715	0.4154878	-1.3371119
H	-3.5260328	0.0922299	-0.3780447
C	-2.8901180	-0.0230556	-2.3414542
O	-1.9463139	-0.7940165	-2.0510771
C	-3.2330163	0.4972972	-3.6186698
C	-4.3268483	1.3491399	-3.8020623
N	-4.4744558	1.6981484	-5.1092816
C	-3.4671544	1.0564791	-5.7344463
H	-3.2736382	1.1062233	-6.7979579
N	-2.7005181	0.3200829	-4.8890627
H	-1.8655129	-0.2426993	-5.1342025
H	-5.8760749	2.3946722	-2.8573088
N	-3.9707527	4.6012116	0.1975363
C	-3.2623496	3.8503715	1.1158402
O	-3.4929738	3.8969442	2.3366698
N	-2.2825246	3.0162162	0.5833311
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C	-1.8886864	2.8934962	-0.7555071
O	-0.9980319	2.0671071	-1.0721970
C	-2.6279159	3.7455453	-1.6186173
C	-3.6646857	4.5550265	-1.1437525
N	-4.2804256	5.2241270	-2.1572398
C	-3.6102138	4.8328126	-3.2592926
H	-3.8250207	5.1758767	-4.2633930
N	-2.6157600	3.9467131	-2.9923743
H	-1.9564320	3.5263779	-3.6743019
H	-4.7010290	5.2159950	0.5484119
N	1.4853838	-6.3851802	-3.6561521
C	0.3233212	-5.6613583	-3.8548551
O	-0.0396912	-5.2785160	-4.9814253
N	-0.3996129	-5.3598912	-2.7064628
H	-1.2687803	-4.8064321	-2.8386894
C	-0.0754780	-5.6602324	-1.3765581
O	-0.8002683	-5.2315246	-0.4462446
C	1.1161690	-6.4242169	-1.2689303
C	1.8788601	-6.7631049	-2.3899787
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C	2.9283774	-7.5309081	-0.6986430
H	3.6632518	-8.0211967	-0.0729810

N	1.8183877	-6.9383877	-0.1881720
H	1.5393490	-6.8836636	0.8073612
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N	1.5330315	-2.3930270	-5.2672320
C	0.3691553	-1.8054391	-4.8056410
O	-0.4024056	-1.1803139	-5.5531331
N	0.1195050	-1.9505511	-3.4451825
H	-0.7373657	-1.4927113	-3.0737783
C	0.9422322	-2.5372164	-2.4726056
O	0.5866997	-2.5323991	-1.2712095
C	2.1246246	-3.0924867	-3.0321909
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H	4.9474917	-4.6386042	-3.3802896
N	3.1933839	-3.7923193	-2.4873857
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H	1.7420103	-2.3155656	-6.2593003
N	1.0847287	1.8109546	-5.6471683
C	0.1744344	2.1270700	-4.6570477
O	-0.8320665	2.8241840	-4.8734390
N	0.4444417	1.5945043	-3.3989917
H	-0.2121477	1.8485839	-2.6363711
C	1.5519245	0.8324122	-3.0043572
O	1.6266696	0.4000077	-1.8280830
C	2.4649740	0.6106996	-4.0698212
C	2.2097555	1.0692771	-5.3660153
N	3.1795545	0.6736792	-6.2361051
C	4.0420060	-0.0207186	-5.4675388
H	4.9517178	-0.4833923	-5.8287390
N	3.6588311	-0.0917097	-4.1661700
H	4.1718972	-0.5510691	-3.3901912
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O	6.2525716	8.8615259	-4.5304756
O	1.6623674	9.1523354	-4.4791153
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C	4.0689060	13.1828361	-4.5979077
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F	2.0250483	14.5413155	-4.6407249
H	4.8345615	13.9413495	-4.6734613
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H	7.7434687	8.2356658	-7.9330977
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O	3.2557722	7.7575144	-10.4715778
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C	7.3694674	9.0431207	-11.0916900
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