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Research Article

Behavior of the Chemicals in the Brain in Viewpoint of Learning Cognition by a Theoretical Simulation

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Abstract

This investigation aims to provide an account of language development in terms of the brain neurochemical transmitters such as dopamine that conducts human speech mechanism using theoretical methods. Brain neurochemical transmitters are effective in language processing, so this work aims to provide an account of language development in terms of the brain neurochemical transmitters such as dopamine that conducts human speech mechanism using theoretical methods. The neurochemical structures of dopamine, epinephrine, norepinephrine, histamine and serotonin have been simulated by Monte Carlo method (MC) which uses the increased temperature to the potential energy of the neurochemicals in the brain considering the geometry optimization of the compounds as an additional conformational level.

It was suggested that dopamine can have a special impact on part of learning language by discussion of IR spectra and MC simulation through the measurement of potential energy in water by increasing the temperature. The results of dopamine nanotube pathway by running the physicochemical parameters as a practical model using Gaussian 09 program package and Multifunctional Wave-function Analyzer can approve the twisting of language-brain due to neurochemical transmitters and nanotubes as density electron deliverers. Theoretical properties of Lagrangian kinetic energy G(r), Hamiltonian kinetic energy, Potential Energy density, Laplacian of electron density; Localized orbital locator (LOL); Local information entropy; average local ionization energy; ESP from nuclear charge; ESP from electrons and Total ESP have been calculated on the dopamine, dopamine with N jointed to BNNT and O jointed to BNNT as neurochemical transmitters.

The most stable of dopamine N or O jointed to BNNT has been approve the best optimized position for localizing the structure through delivery technique in the brain to activate the center of learning language as a simulated model. So, the best results with the calculated amounts and leads us to analyze the perspective of language learning process and enhancing this ability.

Keywords: Language; Neurochemical transmitters; Serotonin; Epinephrine; Norepinephrine; Histamine; Dopamine; BNNT complex; DFT; LOL; G(r); Brain

Introduction

Transferring the chemical messaging in the brain permits daily functions such as thinking, learning, movements, speaking, listening and other activities due to communicating the brain with itself which sends out the chemical information from one neuron or nerve cell to another. Communicating among the human has been investigated by discovering the neuro chemicals in the human's brain to perceive chemical changes produced by people activities and experience.

MR spectroscopic (magnetic resonance) has introduced an account how the children and adults brain develop. Neurochemicals through MR spectroscopy have allowed researchers to study disease processes and mutagenic evolution of subjects in vivo. They have approved that there is a complex association between structural brain development and changes in levels of metabolites, which are organic compounds used or produced by metabolism [1-3].

They have discovered there are several paths for exploring the cognitive domain that cross different subjects' borders and prepare unique outlook on language processing. The attempt to integrate the linguistic perspectives with neurological issues has just commenced to ameliorate the understanding of cerebral mechanisms for language due to the usage of imaging methods and chemical alteration [3].

Neurological experiments have illustrated a central part of function by dopamine in a proper motor commands, learning and higher-order cognitive process with language institute [4-10]. It has been also found that the human has the most improved susceptibility for producing different languages [11-14]. The neuroscience learning through condition changes of brain has been discovered by scientists [15-17]. The grammar knowledge due to a vivid neurophysiological study has been concentrated [18,19].

The structure of brain can be renewed by altering its role for reacting to cognition, environmental reactions or behavioral experience. It has been approved that learning a foreign language changes the structure and function of the brain to be more adaptable and releasing neurochemicals can help powerful learning. So, the most significant interdisciplinary issues of anthropology cognitive science, neurobiology, and chemical interdisciplinary science are produced by language procedures and brain [20].

There are some characteristics of the dopaminergic system consisting of brain systems, domain general functions language functions and related genes. These characteristics can construct the basis for improving informed hypotheses about the genetic fundamental of grammar cognition and memory [21,22] (Figure 1).

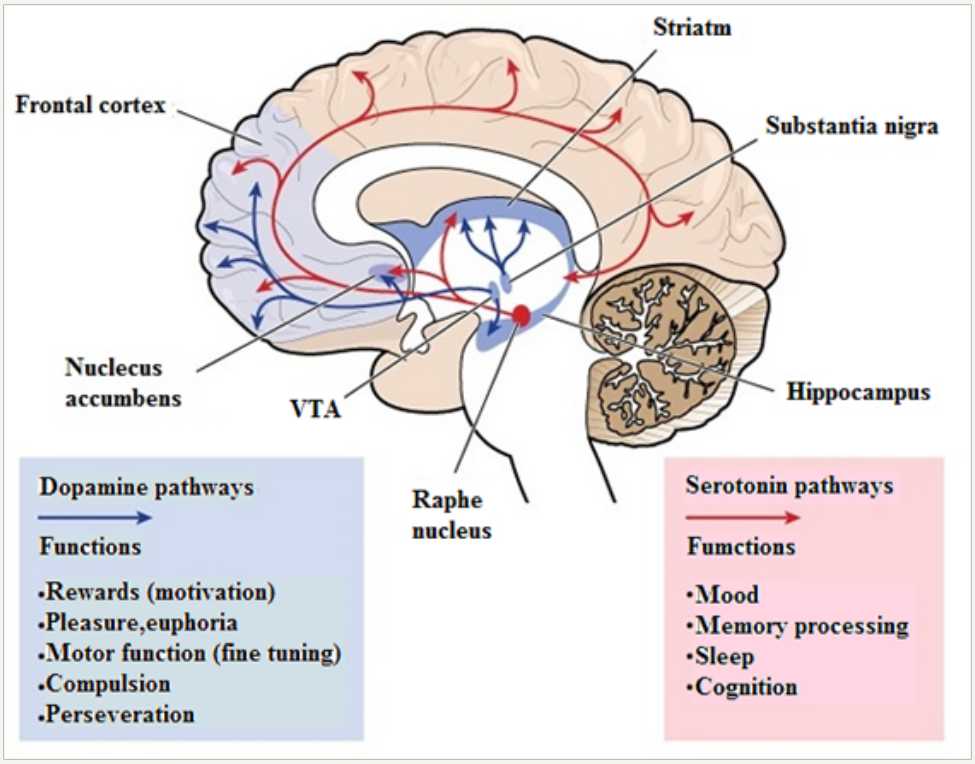

Figure 1: The Brain shows the pathway of two neurotransmitters; dopamine and serotonin through different affection.

The procedure of dopaminergic deals with brain structures [23], procedural memory level [24] but encoded dopamine DA gene receptors and deliverers in nonlinguistic elements are connected to various brain answers and learning rules [25]. In this work, as dopamine is one of the most significant neurochemicals for the learning, a basic part to make motivation to translate the positive understanding and also negative attitudes which reduce dopamine, it has been done a theoretical investigation of founding the Nano structure for injecting dopamine in the brain to enhance its yield as a practical model. In fact, dopamine affects the learning, attention, behavior, cognition, motivation and is jointed with creativity and sociability.

There are some special functions in the brain monitors by monitoring the flow of information from other areas of the brain with the happiness and satisfaction of the brain through reinforcement and enjoyment to persuade us to do activities based on neurobiological theories. Besides, dopamine includes the information flowing to the brain due to learning and conducting the expertise of human.

Dopamine has various feelings and manners due to its chemical effects beside to other neurotransmitters of epinephrine, norepinephrine, histamine and seretonin. Learning is a satisfying and excited for all people (young or adults), so the amount of dopamine increases in the brain to take our information. On the other hand, some learners cannot keep the new knowledge and lose them through the lack of dopamine. The amount of dopamine increases by encouraging students and generates excitement to learn and remember the categorized data in their brain.

In this investigation, it has been studied the interaction between nanostructures (boron nitrogen nanotube) and neurochemicals of dopamine, epinephrine, norepinephrine, histamine and serotonin for discovering immense chemical properties such a simulated model. BNNTs of boron and nitrogen atoms in graphite like structure including are polar in nature. So, electrostatic interactions have an important role for gaining the elastic properties of BNNTs [26,27].

Theoretical Background

The theoretical properties show a variety of parameters of electron structures which are calculated by the method of wave

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function analysis [28,29]. Multiwfn software is suitable for the visual study of real space functions like ELF (electron localization function) and ESP (electrostatic potential) [30]. Also, there is some wave function analysis software limited to the principal analysis methods. The electron density surface of the Dopamine jointed to SWBNNT has been calculated as [31-36]: $\rho(r)=\eta_i|\varphi_i(r)|^2=\Sigma\eta_i\left|\sum_l C_{l,i}\chi_l(r)\right|$ is occupation number of orbital i, is the basis function, ϕ is orbital wave function , and C is Bader which explains the zones by large electron localization include enormous Fermi-hole parameter with a six-dimension function. Probability of spin conditional pair as the spherically averaged has a direct correlation with Fermi hole and the electron localization function [30,37]. ELF(r)= $\frac{1}{1+[D(r)/D_{0(r)}]^2}$, D(r)= , $\frac{1}{2}\sum_i\eta_i|\nabla\varphi_i|^2-\frac{1}{8}[\frac{|\nabla\rho_\alpha|^2}{\rho_\alpha(r)}+\frac{|\nabla\rho_\beta|^2}{\beta(r)}]$, $D_{0(r)}=\frac{3}{10}(6\pi^2)^{\frac{2}{3}}[\rho_\alpha(r)^{\frac{5}{3}}+\rho_\beta(r)^{\frac{5}{3}}]$ Kinetic energy illustrates ELF for post HF wave function and Kohn Sham DFT wave function [38]. Thomas-Fermi kinetic energy density is D0(r) and D(r) indicates the excess kinetic energy density of Pauli repulsion. In fact, a correction value of 10^{-5} to D(r) is shown by Multiwfn program and kinetic energy term changes by Kirzhnits type second order gradient expansion: $\frac{1}{2}\sum_i\eta_i|\nabla\varphi_i|^2\approx D_0(r)+\frac{1}{72}\frac{|\nabla\rho|^2}{\rho(r)+\frac{1}{6}\nabla^2\rho(r)}$. ELF is totally free of the wave-function and can be used to discuss electron density from X-ray diffraction results. Besides, LOL (localized orbital locator) is used for placing high localization areas. LOL has an expression and specified significant chemical zones; it is also comparable to ELF. It has been obtained LOL includes more clear and certain values than ELF [38-42]. LOL can also be explained as a localized orbital, however is has LOL with the kinetic energy like ELF.

In this study, the computational methods have been done using Gaussian 09 on the 8, 0- zigzag dopamine BNNT complexes [43]. The calculated parameters have been done by density functional theory and the Kohn-Sham equation in a plane-wave set with the projector increased wave pseudo-potentials [44-46]. Simulation indicates the methods which aim producing a representative sampling of a system at a finite temperature which calculate most of properties from the partition function [47].

Monte Carlo (MC) force fields that are often used in simulating physical and mathematical systems are class of computational algorithms relying on repeated random sampling to compute their results. Stanislav Ulam and John von Neumann, two physicists, have introduced the Monte Carlo method in the 1940s working on nuclear weapon projects in the Los Alamos National Laboratory to calculate path of neutrons through deuterium and tritium. Monte Carlo method is a statistical sampling technique that over the years has been used successfully to solve a number of scientific questions. Although the computer codes that implement Monte Carlo have grown ever more sophisticated, the essence of the method is captured in some unpublished remarks Stan made in 1983 about solitaire.

MC method is a class of computational algorithms that is based on repeated random sampling to estimate the results which is often applied in simulating physical and mathematical systems. Computation of random or pseudo-random numbers causes the accuracy of calculation especially for unfeasible or impossible to compute an exact result with a deterministic algorithm [48].

It doesn't always need random numbers to use deterministic, pseudo-random sequences, making it easy to test and re-run simulations [49]. In Monte Carlo (MC) methods, a sequence of points in phase space is generated from an initial geometry by adding a random "kick" to the coordinates of a randomly chosen particle (atom or molecule). The new configuration is accepted if the energy decreases and with a probability of e−ΔE/kT if the energy increases. This Metropolis procedure ensures that the configurations in the ensemble obey a Boltzmann distribution, and the possibility of accepting higher energy configurations allows MC methods to climb uphill and escape from a local minimum [49].

Monte Carlo simulations are widely used in the fields of chemistry, biology, physics, and engineering in order to determine the structural and thermodynamic properties of complex systems at the atomic level. Thermodynamic averages of molecular properties can be determined from Monte Carlo methods, as can minimum-energy structures.

MC simulations require only the ability to evaluate the energy of the system, which may be advantageous if calculating the first derivative is difficult or time- consuming. Furthermore, since only a single particle is moved in each step, only the energy changes associated with this move must be calculated, not the total energy for the whole system. A disadvantage of MC methods is the lack of the time dimension and atomic velocities, and they are therefore not suitable for studying time-dependent phenomena or properties depending on momentum [49].

Results and Discussion

The neurochemical compounds of dopamine, epinephrine, norepinephrine, histamine and serotonin have been modeled using computational and theoretical methods to estimate physicochemical properties. The results have shown that dopamine has the lowest optimized energy and the most stabilized structure compared to some other neurochemical transmitters, epinephrine, norepinephrine, histamine and serotonin (Table 1).

Table 1: Thermodynamic properties of neurochemical transmitters in the brain.

Chemical Properties	Dopamine	Epinephrine	Norepinephrine	Histamine	Serotonin
Total Energy (kcal/mol)	-49799.55109	-53245.91911	-49552.7774	-27193.42433	-28007.19049
Binding Energy (kcal/mol)	-2310.425828	-2588.765914	-2063.652136	-750.551744	-1564.317903
Isolated Atomic Energy (kcal/mol)	-47489.12526	-50657.1532	-47489.12526	-26442.87259	-26442.87259
Electronic Energy (kcal/mol)	-260973.313	-294650.4647	-241690.5181	-107649.2927	-133886.5706

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Core-Core Interaction (kcal/mol)	211173.7619	241404.5456	192137.7407	80455.86832	105879.3802
Heat of Formation (kcal/mol)	-78.5068276	-81.7529139	168.2668636	911.816256	98.0500973
Gradient (kcal/mol/Ang)	16.6488558	14.5790881	46.2273058	59.7025527	91.843519

It exhibits dopamine has role the most charge diffusion in the brain (Table 1). Dopamine is not only a neurochemical transmitter released by the brain in humans and other animals, but also has some noteworthy roles such as "cognition", "memory", "behavior", "learning" and etc.

So, it has been perform a vibrational calculation with its own eigenvector and then does the transition state search to find thermodynamic values of neurochemical transmitter such as Total Energy, Binding Energy, Isolated Atomic Energy, Electronic Energy, Core-Core Interaction, Heat of Formation, and Gradient-C.I have been gained (Figure 2).

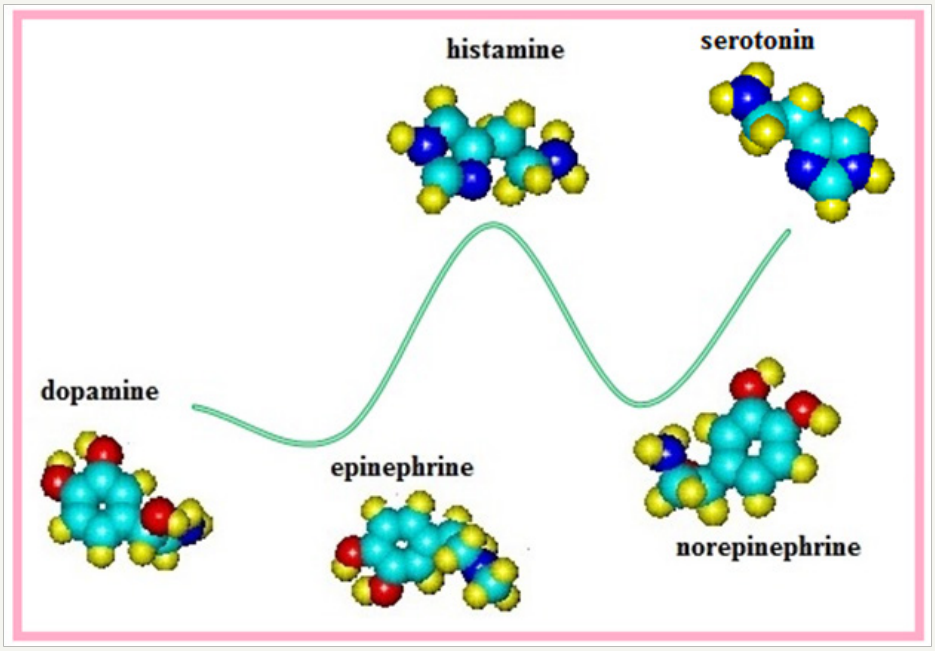

Figure 2: Relative energy (kcal/mol) of some chemical neurotransmitters using IR calculation.

It have been gotten IR technique, infrared radiation, to understand how dopamine does its duties in the brain via three active parts of Nitrogen -Hydrogen, Oxygen-Hydrogen, and benzene structure (Figure 3). Then, surface geometry coordination (x,y,z) for junction of dopamine to zigzag BNNT complex as dopamine-nanotube neurotransmitter (N and O active sites) for structure of model (Table 2 and Figure 4a-4d).

Table 2: Geometry coordination (x,y,z) for junction of dopamine to zigzag BNNT complex as dopamine-nanotube neurotransmitter (N and O active sites).

Atoms	x(N)	y(N)	z(N)	x(O)	y(O)	z(O)
01	-14.7858	-0.6044	3.0776	-13.9325	-1.9094	-1.6848
08	-14.3237	4.4399	2.8761	-14.8947	3.1596	-2.3082
014	-8.7279	-4.3293	-3.3103	-4.7514	-2.0413	0.7839

Also, Some properties such as density of all electron; Lagrangian kinetic energy G(r), Hamiltonian kinetic energy, Potential Energy density, Laplacian of electron density; Localized orbital locator (LOL); Local information entropy; average local ionization energy; ESP from nuclear charge; ESP from electrons and Total ESP have been calculated on the dopamine (Table 3a and Figure 5a & 5b), dopamine with N jointed to BNNT (Table 3b) and O jointed to BNNT (Table 3c) as neurochemical transmitters using the Multifunctional Wave function Analyzer [40-42] (Table 3 and Figure 6a-6c) .

Table 3b & 3c show two sites of N and O atoms from dopamine molecule which linked to BNNT (Figure 6a-6c). Theoretical properties of density of all electron, density alpha electron and Hamiltonian kinetic energy, Local information entropy, ESP from electrons (Figure 5a), Lagrangian kinetic energy, Potential density, Laplacian of electron density (Figure 5b) for dopamine and Lagrangian kinetic energy G(r), potential energy density V(r), Laplacian of electron density (LED) for dopamine-BNNT complex have been plotted due to N and O linkages, respectively (Figure 6a-6c).

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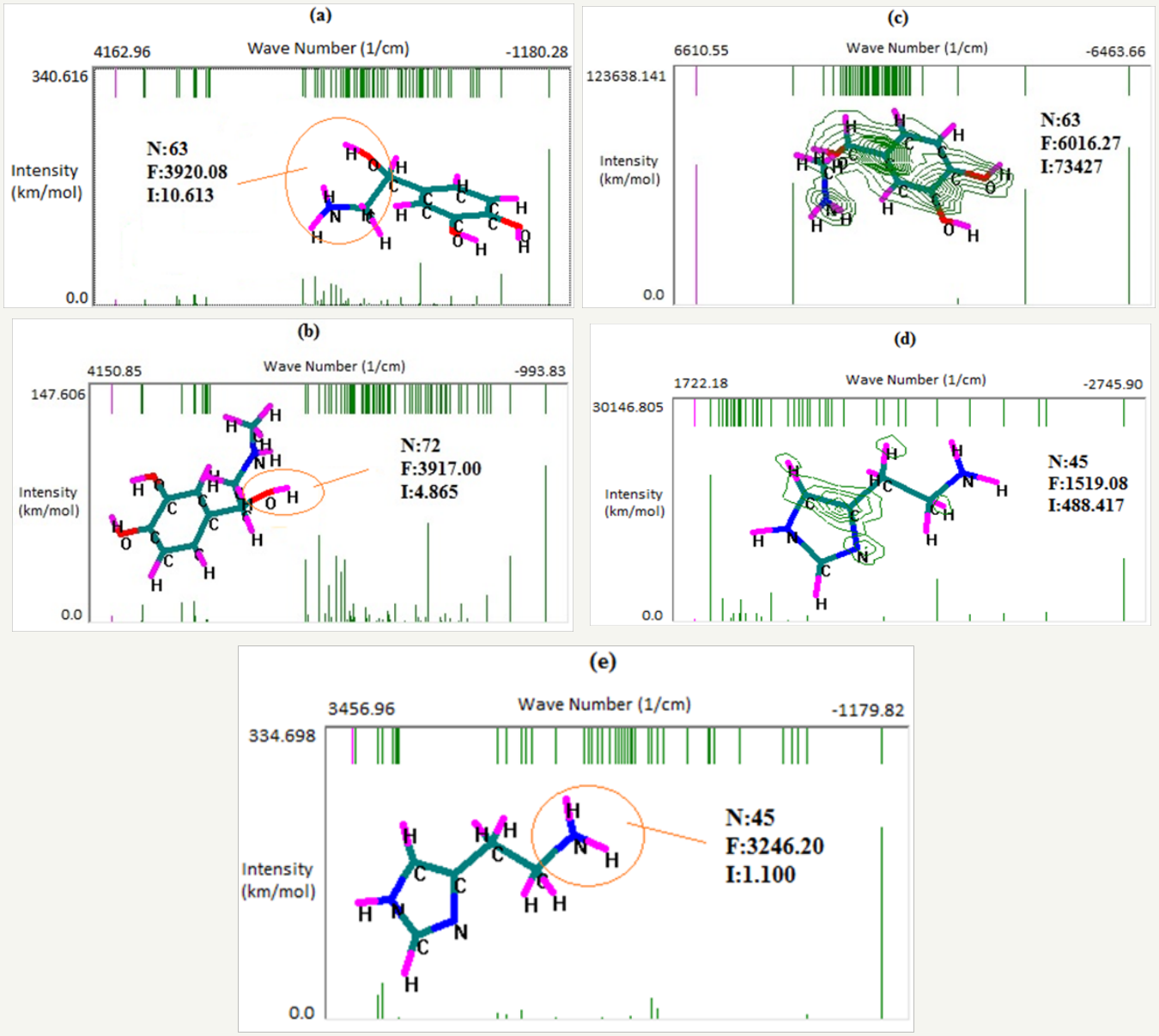

Figure 3: IR spectra of neurochemical transmitters of (a) dopamine (b)epinephrine (c) norepinephrine (d) histamine and (e) serotonin.

Obviously, more stable of dopamine with N or O linked to BNNT has been investigated the best coordination for citing the structure using delivery technique in the brain to promote the center of learning language as a model (Table 3b & 3c and Figure 6a-6c).

Then, dopamine, epinephrine, norepinephrine, histamine and seretonin have led to a description of Monte Carlo (MC) simulation by potential energy in 300K energy via time scale (0-100) by Monte Carlo method (Figure 7). Optimal values are close to 0.5. Varying the step size can have a large effect on the acceptance ratio. The Monte Carlo Options dialog box permits us to set up the MC simulation parameters. In this work, it has been run a temperature simulation with 100 steps.

Moreover, in Figure 8a-8f , it has been seen the changes of potential energy vs. time scale and different temperatures of 305,310,315 and 320K for dopamine with max delta and time steps of 0.05 Å, 1, respectively (the order of polynomial line is 6) (Table 4). Study of the solution state has invoked much interest among investigators and a lot has been done in the study of solute-solvent interactions. Water is the main solvent environment for a majority of biomolecules. It has been estimated the potential of dopamine with a simulated model of solute-solvent of dopamine-water in a periodic box (X,Y,Z=18.70136Å with maximum number of water molecule 216, minimum distance between solvent and solute molecules 2.3Å) using program package HyperChem 8 [50] (Figure 9).

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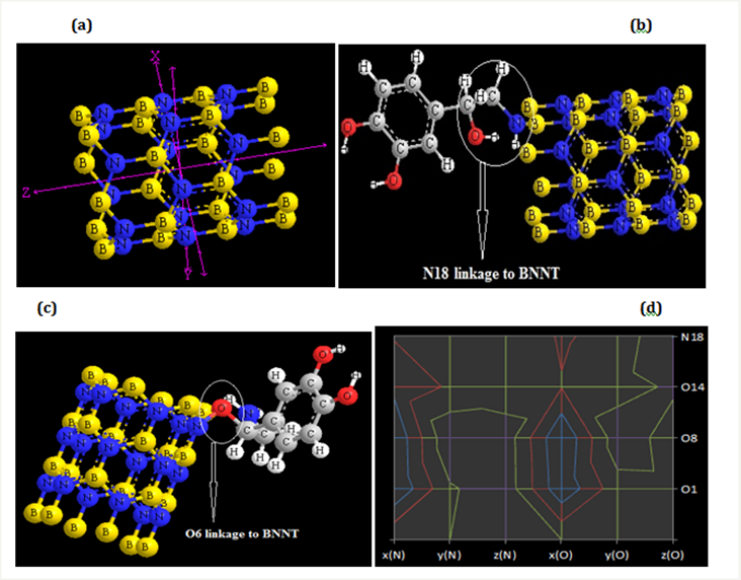

Figure 4:

4a: Boron Nitride Nanotube with Inertial Axes, dopamine- BNNT deliverer of different citations of

4b: N18

4c: O6 linkage as the optimized models and S

4d: Surface geometry coordination (x,y,z) for junction of dopamine to zigzag BNNT complex as dopamine-nanotube neurotransmitter (N and O active sites).

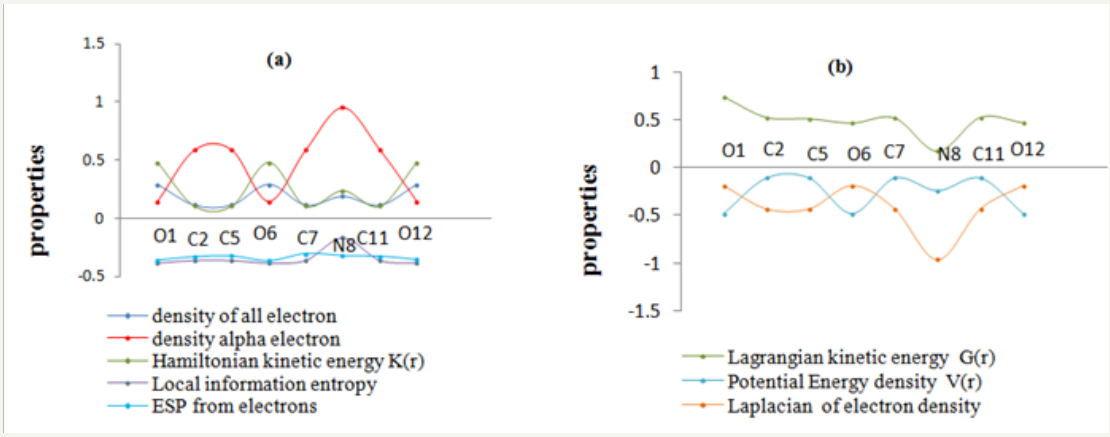

Figure 5: Theoretical properties of

5a: Density of all electron, density alpha electron and Hamiltonian kinetic energy, Local information entropy, ESP from electrons

5b: Lagrangian kinetic energy, Potential density, Laplacian of electron density for dopamine as a Nano transmitter in the brain.

It has been shown the potential energy graph of dopamine in solvent via time scale (0-100) in 300K using Monte Carlo method (Max delta =0.05Å, time steps=1) by polynomial (order=6) (Figure 10a) and has been Compared the potential energy of dopamine and dopamine-water through the relation coefficient factor (R) in two media. It has been gained R-squared value on chart as; R2=0.8888 for dopamine and R2=0.6656 for dopamine- H2O (Figure 10b).

The results of the above observations strongly suggest that the different data observed in the dopamine in the solvent is predominantly due basis set functions, induced by a change in polarity of the environment. It is clear that an increase in the dielectric constants increases the stability of dopamine (Figure 10).

Conclusion

The power of language learning produced by chemical neurotransmitters in the brain has been studied. Linkage of dopamine on the edge of (8,0) zigzag BNNT is modeled in different positions through transferring the electron. BNNT is a

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steady structure for delivery of dopamine that depends on the coordination of atoms interaction in the complex. These electrons can be distinguished by the citing and other quantum mechanical properties. The jointed atoms of nitrogen and oxygen by large electron localization and magnitudes of Fermi-hole integration have been approved through considering the spherical average of the spin for the Fermi hole [30].

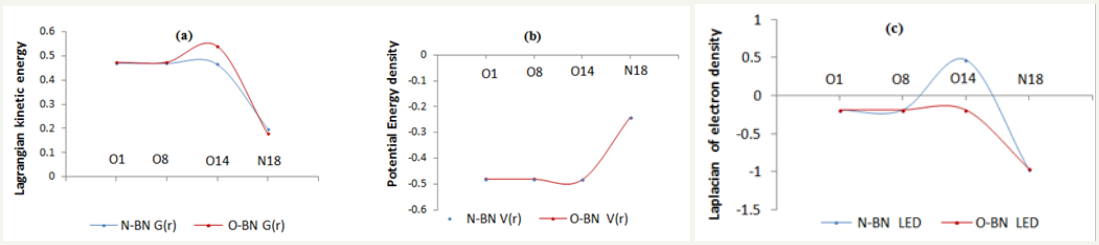

Figure 6:

6a: Lagrangian kinetic energy G(r)

6b: Potenitial energy density V(r) and

6c: Laplacian of electron density via active atoms of Nitrogen and Oxygen formed the complex of N-BN and O-BN).

Table 3: Calculated properties on

Atoms	Density of All Electron	Density Alpha Electron	Lagrangian Kinetic Energy G(r)	Hamiltonian Kinetic Energy K(r)	Potential Energy Density V(r)	Laplacian of Electron Density	Localized Orbital Locator (LOL)	Local Information Entropy	Average Local Ionization Energy	ESP from Electrons	Total ESP
(a)											
O1	0.2909	0.1454	0.7402	0.4813	-0.4814	-0.1925	0.9987	-0.3791	0.1834	-0.356	0.9644
C2	0.1181	0.5904	0.5244	0.1091	-0.1091	-0.4364	0.9993	-0.3562	0.9915	-0.3272	0.9673
C5	0.1181	0.5905	0.5117	0.1092	-0.1092	-0.4367	0.9993	-0.3567	0.99	-0.32	0.968
O6	0.291	0.1455	0.466	0.4816	-0.4816	-0.1926	0.9987	-0.3795	0.1827	-0.3615	0.9638
C7	0.1181	0.5904	0.5179	0.1091	-0.1091	-0.4366	0.9993	-0.3563	0.9887	-0.3002	0.9699
N8	0.1913	0.9564	0.1742	0.2414	-0.2414	-0.9657	0.999	-0.1602	0.138	-0.3182	0.9682
C11	0.1181	0.5903	0.5253	0.1091	-0.1091	-0.4364	0.9993	-0.3561	0.991	-0.323	0.9677
O12	0.2909	0.1455	0.4692	0.4815	-0.4815	-0.1926	0.9987	-0.3793	0.1832	-0.3515	0.9648
(b)											
O1	0.2909	0.1454	0.4701	0.4814	-0.4814	-0.1925	0.9987	0.1226	0.1836	-0.4867	0.9513
O8	0.2909	0.1454	0.4691	0.4815	-0.4815	-0.1926	0.9987	0.1224	0.1833	-0.481	0.9519
O14	0.2911	0.1455	0.465	0.4817	-0.4817	0.465	0.9987	0.1221	0.1831	-0.542	0.9458
N18	0.1925	0.9625	0.198	0.2432	-0.2432	-0.9727	0.9989	0.3183	0.1374	-0.611	0.9389
(c)											
O1	0.2908	0.1454	0.4741	0.4812	-0.4813	-0.1925	0.9987	0.1227	0.1837	-0.4983	0.9501
O8	0.2908	0.1454	0.4739	0.4812	-0.4813	-0.1925	0.9987	0.1227	0.1837	-0.4831	0.9517
O14	0.2921	0.1461	0.54	0.4835	-0.4836	-0.1943	0.9985	0.1195	0.1835	-0.6699	0.933
N18	0.1911	0.9553	0.179	0.2412	-0.2412	-0.9646	0.999	0.3202	0.1382	-0.5392	0.9461

3a: Dopamine

3b: 8,0 zigzag dopamine BNNT deliverer in the brain due to N linkage

3c: 8,0 zigzag dopamine BNNT deliverer in the brain due to O linkage.

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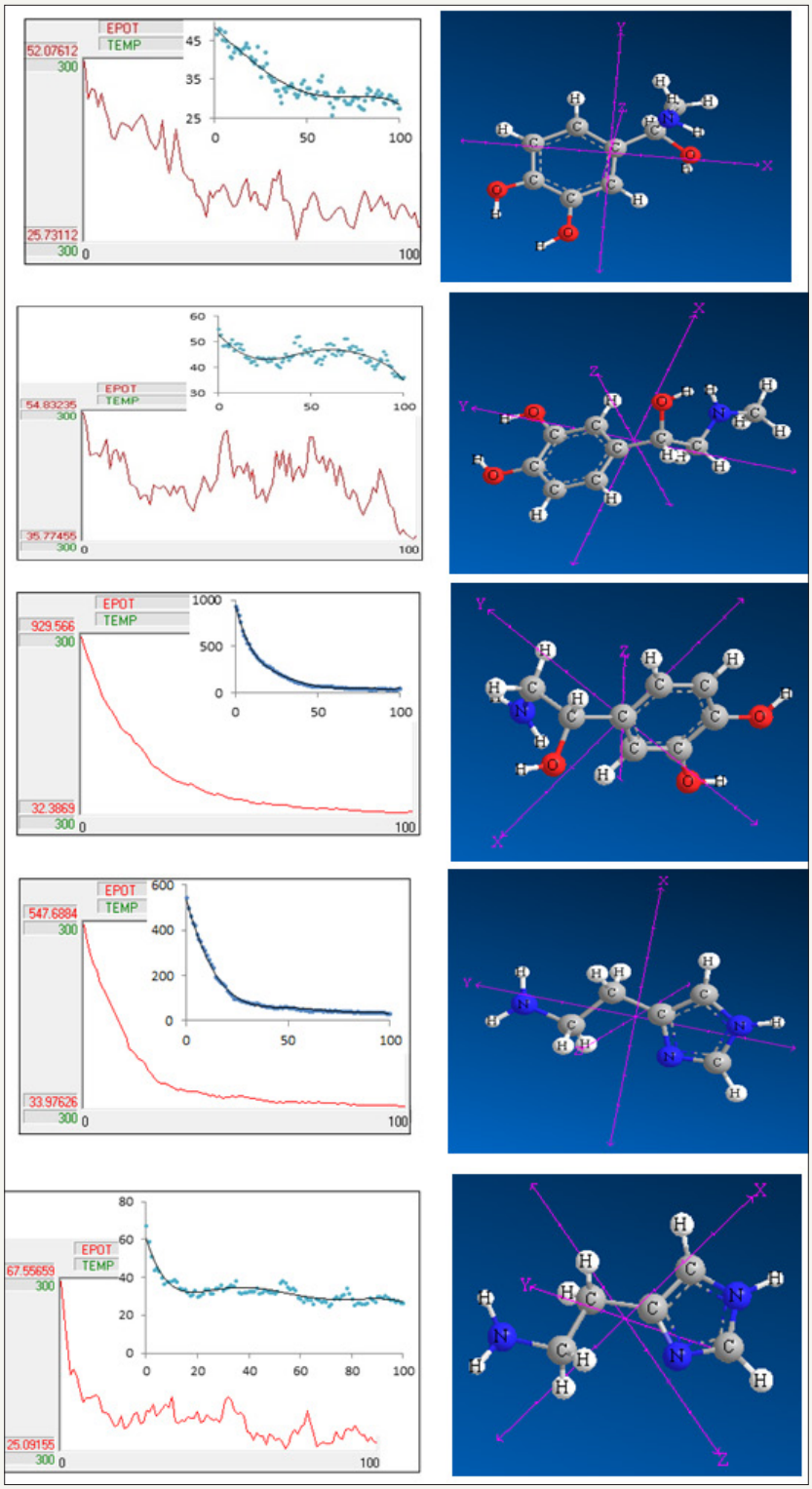

Figure 7: Calculated potential energy graphs of

7a: Dopamine

7b: Epinephrine

7c: Norepinephrine

7d: Histamine and

7e: Serotonin via time scale (0-100) by Monte Carlo method.

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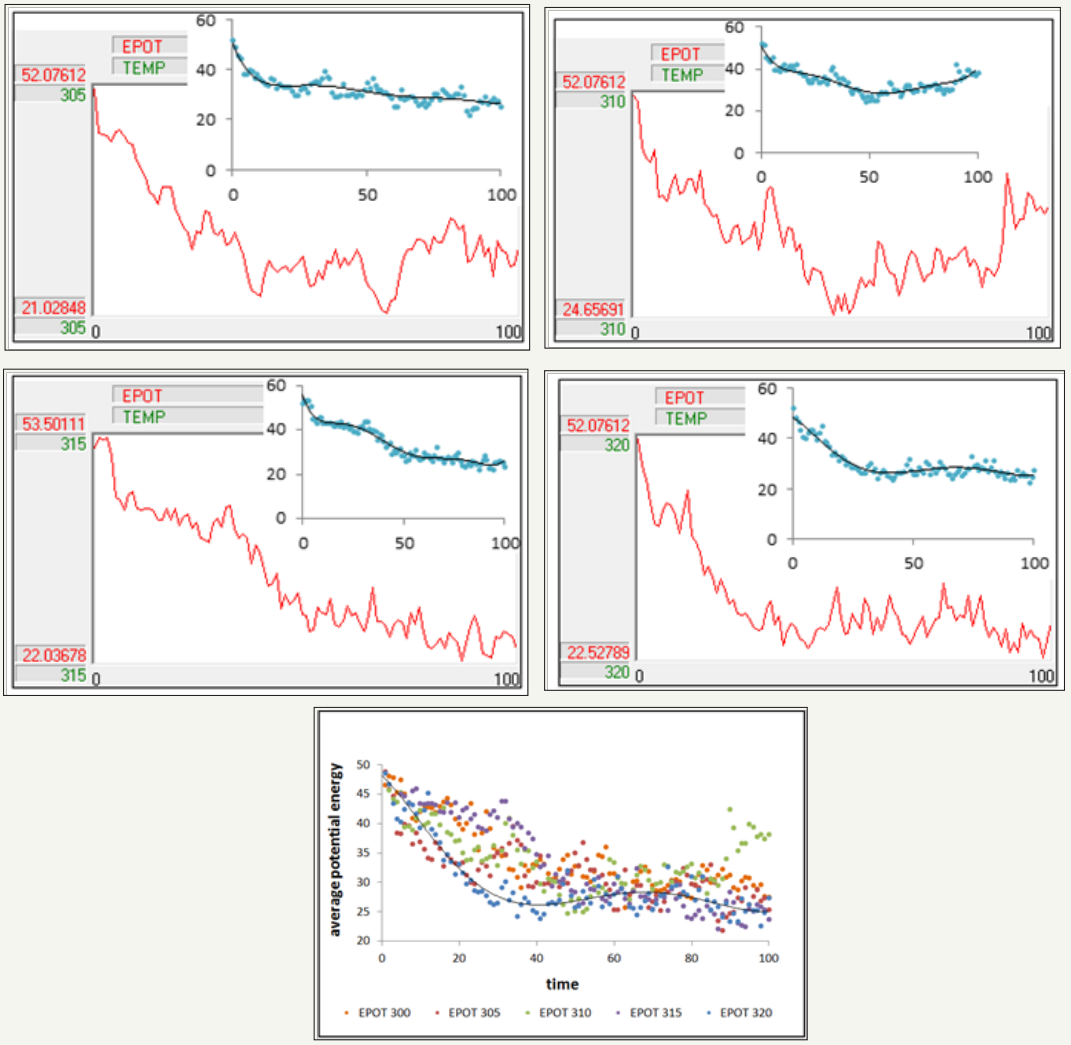

Figure 8:

8a-8d: Calculated potential energy graphs of dopamine via temperatures by Monte Carlo method and

8e: Average potential energy for dopamine in 300- 320 K using MC force filed.

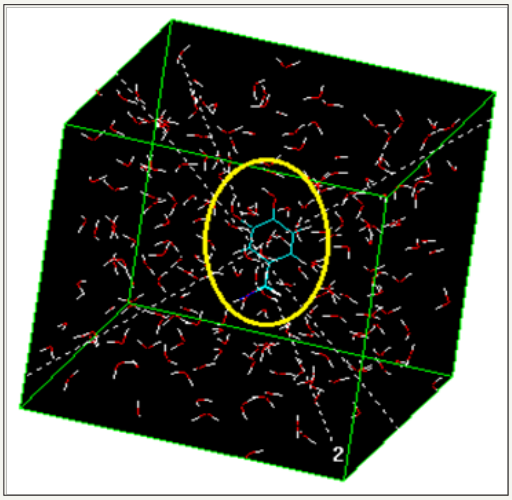

Figure 9: A simulated model of solute-solvent of dopamine-water in a periodic box (X,Y,Z=18.70136Å, maximum number of water molecule 216, minimum distance between solvent and solute molecules 2.3Å).

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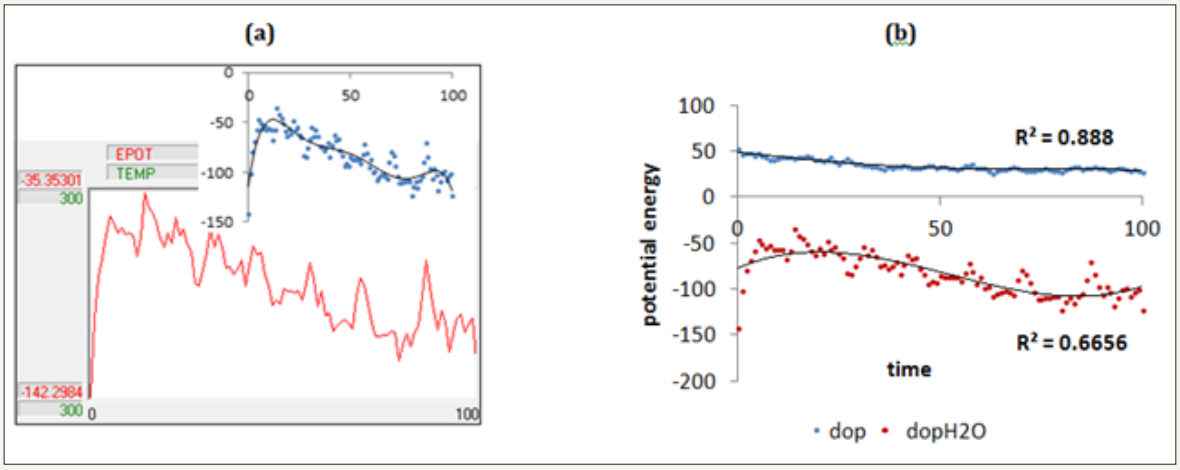

Figure 10:

10a: Calculated potential energy graphs of dopamine in the periodic box via time scale (0-100) in different temperatures by Monte Carlo method and

10b: Comparison between the potential energy of dopamine and dopamine-water through the relation coefficient factor (R) in two media.

Table 4: The changes of potential energy vs. time scale and different temperatures (K) for dopamine with max delta =0.05Å and time steps=1.

Time	300	305	310	315	320	Time	300	305	310	315	320
0	52.07612	52.07612	52.07612	52.07612	52.07612	51	32.75209	32.85038	27.22954	26.209	25.95078
1	46.6004	48.86794	51.36514	53.4856	48.53438	52	30.93908	36.71789	24.90222	26.50787	28.44804
2	48.0702	45.86107	45.67031	53.21227	46.65721	53	30.83483	33.93947	25.4753	29.67292	27.35468
3	47.85444	44.65378	44.20803	53.50111	43.4069	54	30.13794	32.12197	27.62951	28.86792	26.46304
4	45.33366	38.34203	43.70484	51.00751	40.76036	55	31.88361	32.13003	29.27543	28.69199	30.51553
5	47.42036	38.22336	45.34875	45.11192	40.25707	56	34.67202	30.90939	28.19147	30.85265	29.38553
6	45.09726	39.95332	39.4423	44.65003	42.39537	57	34.43159	31.21923	29.04751	27.21917	25.77525
7	43.55555	39.67263	39.59328	43.37886	43.52078	58	36.07374	29.6897	28.38098	26.82575	27.9828
8	40.96535	36.45863	38.89928	45.56585	43.12489	59	31.53944	28.68232	33.89625	27.60041	26.30645
9	40.52354	38.46413	40.86501	45.95712	41.72498	60	31.5313	25.31282	33.36773	29.73818	28.03574
10	42.02027	36.87225	42.24352	43.48468	39.30553	61	31.04957	25.29148	30.70739	28.39148	30.95438
11	43.11378	35.67336	39.78106	43.31918	42.31678	62	28.98329	28.92036	29.83273	28.82098	28.97442
12	42.78516	34.12247	40.1791	43.4815	45.18411	63	25.73112	32.1231	29.70468	27.18511	28.05086
13	42.64036	33.87194	41.65339	43.45306	39.01018	64	27.8099	27.95514	27.11208	26.2794	25.78436
14	41.89095	36.754	41.6484	43.16214	38.14517	65	30.16283	28.76288	28.66739	28.49391	25.6134
15	42.93142	35.81352	39.84221	42.04878	36.80489	66	30.29309	29.48241	31.20745	32.33697	24.39984
16	43.64935	32.68924	42.63697	41.90928	33.72116	67	31.92164	29.4675	32.69633	27.56083	25.66582
17	44.28754	34.59768	38.5596	43.51405	34.81115	68	32.65779	27.5849	32.12463	27.61957	26.90434
18	43.13892	33.85933	38.08964	41.97584	33.45231	69	31.87786	25.67364	30.31494	27.06272	28.05099
19	40.75792	33.22774	36.98458	43.61633	31.39538	70	29.5283	26.7174	28.83767	25.42771	25.28625
20	39.9257	33.05265	37.18072	41.0966	33.15437	71	28.65976	27.80605	29.69276	27.11733	26.36592
21	39.08829	33.37552	35.03461	42.29409	31.61859	72	28.60217	25.22293	29.94538	27.85165	27.76002
22	40.04858	31.25223	33.74737	42.72393	29.79344	73	28.84434	26.67666	33.01735	27.42595	27.97238
23	43.37444	30.0162	33.94053	40.80353	30.34379	74	29.53469	28.37526	32.70968	25.23418	32.66893
24	38.20774	29.73337	35.52177	41.58904	28.58697	75	30.3099	30.2874	30.06059	28.81435	29.1949
25	35.55247	32.05903	36.02291	39.39991	28.31759	76	30.5398	30.15335	31.68933	27.16693	29.51465
26	38.409	33.42013	33.57673	39.18628	28.48697	77	30.13857	27.95507	31.53465	29.66336	27.56428

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27	42.0568	32.70532	34.06705	38.72065	27.68323	78	28.11983	32.35749	31.92886	25.96541	28.29371
28	39.1405	31.12627	34.33945	41.50486	26.59128	79	27.54953	31.2189	32.61055	24.08536	27.86642
29	35.90638	34.40828	36.30423	42.1605	26.23722	80	27.3469	29.67041	33.14244	23.8389	31.0056
30	35.30422	35.0652	32.87651	41.01405	26.42969	81	29.62173	29.47705	30.78711	24.42507	26.91684
31	34.54963	35.7097	35.39139	43.76746	29.0921	82	31.33262	29.08321	31.58299	25.19845	28.74009
32	34.59335	34.71686	39.98896	43.85863	30.14143	83	32.85518	30.23111	30.76731	23.85774	31.01295
33	32.21888	36.66212	40.92949	40.80231	26.98064	84	32.09736	30.42896	28.15941	25.96734	26.97768
34	32.10555	39.53718	37.98143	39.38261	28.17901	85	29.96411	33.04883	30.63803	25.26202	25.33172
35	30.86633	37.09692	35.57095	40.03991	24.2403	86	30.53918	29.99052	30.19628	24.60867	26.67311
36	29.10934	36.3732	33.09204	39.38529	26.24521	87	31.22088	23.50894	29.52452	22.03678	25.87665
37	32.89454	31.14112	35.52779	35.8175	27.28432	88	32.19732	21.76631	30.61666	24.57759	24.08368
38	31.9761	29.35248	35.39315	38.37387	26.63529	89	30.80939	24.10737	34.00976	26.87968	26.41365
39	32.97184	29.27214	32.55552	37.4132	25.23567	90	31.23676	24.64446	42.36215	28.35475	23.33898
40	32.96017	29.95739	33.48793	34.77733	24.85508	91	29.1209	24.94624	39.22253	26.54021	24.6678
41	33.92505	34.47646	29.70853	32.67645	23.77911	92	28.73569	27.38182	35.33441	23.07501	23.33228
42	33.07223	29.73562	28.47568	32.99222	24.57486	93	30.25096	26.84951	36.64393	22.75637	27.19691
43	31.46126	29.88568	30.61439	34.45315	26.29102	94	30.88824	29.09739	36.62765	22.38784	25.14442
44	30.52735	30.225	30.28958	29.34923	26.58302	95	30.71544	26.22977	39.93041	25.51762	26.26232
45	30.97131	30.38674	30.10831	31.39889	26.33343	96	29.5149	27.62273	39.4561	25.14028	25.25191
46	32.28316	29.24055	27.88686	30.05414	26.97416	97	28.87957	28.72479	37.74101	26.16211	25.17316
47	33.86043	30.30991	26.25641	30.66138	29.69966	98	29.65664	26.85583	38.13234	25.88727	22.52789
48	34.66233	29.85158	24.65692	31.51181	32.02631	99	27.53831	27.3514	37.33766	25.39646	24.88292
49	31.34989	31.97225	27.0043	28.65347	27.6928	100	27.41156	25.36543	38.16652	23.66159	27.3819
50	32.72585	34.95446	25.10595	28.32523	25.69217						

The simulations of dopamine - BNNT show that the stabilization energy has been affected by the Monte Carlo force field and different temperature and the best results have been gained for potential energy vs. temperature at MC force field and by increasing of temperature, our calculations have demonstrated that such extrapolation schemes significantly overestimate the dopamine-BNNT by active site of molecule (N and O linkage) which are the most active point at indicated structure.

This paper can lead us to find how neurochemical transmitters in the brain jointed to nanotubes can be effective act for learning a new language based on simulated model through drug delivery method and theoretical calculations of quantum mechanics [51-53].

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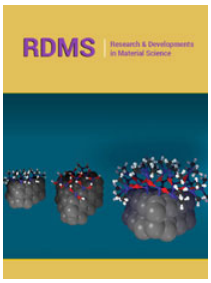

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