Nexo Revista Científica
Vol. 34, No. 02, pp. 776-789/Junio 2021

ISSN-E 1995-9516
Universidad Nacional de Ingeniería

http://revistas.uni.edu.ni/index.php/Nexo
https://doi.org/10.5377/nexo.v34i02.11566

Investigation of different SWCNTs interaction with dopamine and serotonin anticancers: a theoretical study

Investigación de la interacción de diferentes SWCNT con anticancerosos de dopamina y serotonina: un estudio teórico

Nastaran Saghayimarouf [1], Majid Monajjemi[2], Karim Zare*[,1], Ali Shamel[3]

[1]Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran.
[2]Department of Chemical Engineering, Central Tehran Branch, Islamic Azad University, Tehran, Iran.
[3]Department of Chemistry, Ardabil Branch, Islamic Azad University, Ardabil, Iran.

k-zare@srbiau.ac.ir

(recibido/received: 14-octubre-2020; aceptado/accepted: 27-enero-2021)

ABSTRACT

Carbon nano tubes (CNTS) have two basic structure as single-walled and multi-walled based on hexagonal plexus of carbon atoms. CNTs can serve as platforms to conjugate other compounds specially in medications purposes by immobilization of biomolecules at their surface. Dopamine and serotonin are two biological molecules which have bifunctional activities as hormone and neurotransmitter. These two molecules have important roles as neurotransmitters in the central and peripheral nervous systems but serotonin functions as a mood regulator, while dopamine is connected to the "pleasure center". In this article we optimized molecular and structural properties of connected dopamine and serotonin with SWNTS with four different diameters (7.0,7.5,7.7 and 10.0 nm) by using molecular quantum methods such as NMR shielding tensor data by B3LYP level of theory with 6-31 G(d) as a basis set, mk and frequency methods. Theoretical computations were performed to study NMR chemical shift data including magnetic shielding tensor (σ, ppm), shielding asymmetry (η), magnetic shielding anisotropy (σaniso), magnetic shielding isotropy (σiso) , skew of a tensor (K) and chemical shift anisotropy (Δσ) and span (Ω) at various rotation angles around a specific rotation , physical and chemical properties of atomic nuclei , frequency data by B3LYP/6-31g level of theory and POP method using gaussian 09 program.

Keywords: Dopamine, Serotonin, SWCNTs, NMR, Frequency.

RESUMEN

Los nanotubos de carbono (CNTS) tienen dos estructuras básicas como de pared simple y de pared múltiple basadas en plexos hexagonales de átomos de carbono. Los CNT pueden servir como plataformas para conjugar otros compuestos especialmente en medicamentos mediante la inmovilización de biomoléculas en su superficie. La dopamina y la serotonina son dos moléculas biológicas que tienen actividades bifuncionales como hormona y neurotransmisor. Estas dos moléculas tienen funciones importantes como neurotransmisores en los sistemas nerviosos central y periférico, pero la serotonina funciona como un regulador del estado de ánimo, mientras que la dopamina está conectada al "centro del placer". En este artículo optimizamos las propiedades moleculares y estructurales de la dopamina y la serotonina conectadas con SWNTS con cuatro diámetros diferentes (7.0, 7.5, 7.7 y 10.0 nm) mediante el uso de métodos cuánticos

moleculares como los datos del tensor de blindaje de RMN mediante el nivel de teoría B3LYP con 6-31 G (d) como conjunto de bases, mk y métodos de frecuencia. Se realizaron cálculos teóricos para estudiar los datos de desplazamiento químico de RMN, incluido el tensor de blindaje magnético (σ, ppm), la asimetría de blindaje (η), la anisotropía de blindaje magnético (σaniso), la isotropía de blindaje magnético (σiso), la desviación de un tensor (K) y el desplazamiento químico anisotropía (Δσ) y span (Ω) en varios ángulos de rotación alrededor de una rotación específica, propiedades físicas y químicas de los núcleos atómicos, datos de frecuencia por nivel de teoría B3LYP / 6-31g y método POP utilizando el programa gaussiano 09.

Palabras clave: Dopamina, Serotonina, SWCNT, RMN, Frecuencia.

1. INTRODUCTION

Dopamine is a medication form of a substance that occurs naturally in the body based on catecholamine and phenethylamine families and suppose to function both as a hormone and a neurotransmitter (Berridge, 2009). Also, it is known as feel good hormone as the secondary messenger system which sends messages between nerve cells in the braaccouin, binds to receptors in the brain and making them send signals from one cell to another and causes cellular changes that can affect your well-being in a number of ways for instant, in moments of pleasure and reward, we get a rush of dopamine, and when levels are too low, we feel a lack of motivation and feelings of helplessness (Romanelli, 2009; Robinson, 1993).

As Dopamine hormonal function can be mentioned as reduces of secretion of prolactin by stimulating theD2 receptors, thereby affecting milk production (Lindemann,2005) and also in memory consolidation, Dopamine or Dopamine agonists have critical role (Wise, 2004).

Abnormal dopamine levels (either too high or too low) are also linked to many pathological disorders, such as Schizophrenia, Tourette's syndrome, Parkinson's disease, Alzheimer's disease, Huntington's disease and Attention deficit hyperactivity disorder (ADHD) (Dickson, 2007; Howes, 2009; Miller, 2011).

Research also highlights that dopamine receptors are found in the kidneys, pancreas, lungs and blood vessels outside the central nervous system and belong to the large family of Heptahelical transmembrane spanning G protein-coupled receptors (GPCRs). By now five mammalian dopamine receptor subtypes have been identified and are classified into two major groups, the D1-like (D_1 and D_5) which are mostly found in the cerebral cortex, hypothalamus, and thalamus and D2-like (D_2, D_3, and D_4) receptors which are similar in structure but differ by their affinity for dopamine and coupling to downstream effectors like G protein. G-protein-coupled receptors also regulate the activity of PKB/Akt (protein kinase B) at serine-473 (Ser473) and threonine-308 (Thr308) although the mechanisms of these functions are poorly understood (Xiangdang, 2010). D3 and D4 receptors are less abundant and less widely distributed compared to D_2 receptors (Romanelli,2009).

The contribution of dopamine receptor subtypes to increase of sensitization behavior in response to AMPH(Amphetamine) has been widely studied by blocking D1 and D2 receptors during repeated AMPH administration. These studies demonstrate an acute role for D1 receptors and D2 receptors as a supporting or secondary role in the development of AMPH sensitization (Vanderschuren, 2000).

Dopamine D_1 or D_2 receptor agonists despite of neurotrophin receptor stimulation, phosphorylate Akt at the Thr308 residue, not via phosphoinositide 3-kinase (PI3K), but via PKA (protein kinase A) and ERK (extracellular signal-regulated kinase) activation in primary striatal cultures (Brami-Cherrier,2002).

Studies show that Signaling through dopamine receptors adjust neurotic processes such as motoractivity, motivation and reward (including drug-seeking behavior), and highercognition (including working memory) (Kienast, 2006).

Dopamine receptors are involved in all of the physiological functions of dopamine such as the autonomic movement, emotion, hormonal regulation, dopamine-induced immune effects, and tumor behavior, and etc. some evidences show that dopamine receptors are associated with the regulation of tumor behavior, including tumor cell death, proliferation, invasion, and migration which cannot only directly affect tumor behavior, but also limit tumor progress via activating tumor immunity (Wang, 2019).

Dopamine and Serotonin have important roles as neurotransmitters in the central and peripheral nervous systems (Deutch,1999) but serotonin functions as a mood regulator, while dopamine is connected to the "pleasure center.".

Serotonin [5-hydroxytryptamine (5-HT)] has an important role in many organs as a peripheral hormone transported by blood platelets and is released upon activation (Berger, 2009; Herr, 2017). This diverse functions of serotonin in the brain are mediated by multiple 5-HT receptor subtypes (15 known subtypes). These subtypes were at first classified based on pure pharmacological criteria ad belong to different families of 5-HT receptors (Peroutka, 1990).5-HT $_2$and 5-HT$_{1c}$ are structurally similar and therefore have similar biochemical activation consequences and pharmacological profile (Conn, 1984; Conn, 1986; Hoyer, 1988). 5-HT$_2$ and 5-HT$_{1c}$ and the new discovered one (5-HT$_{2f}$) which lately renamed as 5-HT$_{2A}$, 5-HT$_{2c}$ and 5-HT$_{2B}$, demonstrated striking protection in their amino acid sequence, thus claimed that they could have evolved by mutation from a common ancestral gene (Julius, 1988).

As a neurotransmitter, serotonin participate in regulation of sleep, appetite, mood, and other important brain functions which cannot cross form blood-brain-barrier and needs transporter. Peripheral serotonin roles are the regulation of logical processes including cardiovascular function, bowel motility, ejaculatory latency, and bladder control, hemostasis, heart rate, intestinal motility, cell growth in liver, bone, and pulmonary arteries, and the development of heart, brain, and mammary gland and some addition roles in immunoregulatory functions including pro-inflammatory functions (Berger, 2009). Pro-inflammatory feature is now known that platelets ensure the targeted release of serotonin in platelet-activating environments like a thrombus or an inflammatory reaction (Wagner, 2008; Endo, 1997; Mössner, 1998).

Contrary to what has been said about the anti-inflammatory properties of serotonin, a specific activation of the 5-HT2A receptor subtype in primary aortic smooth muscle cells causes a superpotent inhibition of tumor necrosis factor (TNF)-α-mediated inflammation (Yu, 2008; Herr, 2017).

Possible sources for peripheral serotonin are plasma, monocytes/macrophages, lymphocytes, vascular smooth muscle cells, adipocytes, mast cells (although human mast cells were long thought not to contain serotonin), and platelets (Herr, 2017).

Nanomaterials possess unique features which make them particularly attractive for biosensing applications.

Carbone nanotubes based on the number of walls, designed as single-walled carbon nanotube and multi-walled carbon nanotube. The side- walls of these tubes are made up of a hexagonal plexus, of carbon atoms, similar to graphene and are usually capped at both ends by one half of a fullerene-like molecule (Zhu, 2002; Tîlmaciu, 2015). Carbon nanotubes (CNTs) can be used as scaffolds for immobilization of biomolecules at their surface and best suited materials for the transduction of signals associated with the recognition of analytes, metabolites, or disease biomarkers due to their several exceptional properties such as physical, chemical, electrical, and optical characteristics properties. Besides CNTs can cross biological barriers including the cell membrane (Tîlmaciu, 2015; Pantarotto, 2004; Monajjemi,2019).

2. Material and Methods

Quantum mechanics (MQ)Calculations were performed using Gaussian 09 to study chemical and physical properties of nuclei (Reed, 1988; Monajjemi, 2020; Monajjemi, 2020). In this work, it has been mainly

focused on optimized structures of combined Dopamine and Serotonin molecule with SWNTs with 7.0, 7.5, 7,7 and 10.0 nanometer diameter in NMR, POP=MK (Merz-Singh-Kollman) and freq methods.

Gaussian 09 uses numerical methods to find solutions to wave functions. Varies methods such as molecular orbital energies, bond energies, molecular geometries and energies, and vibrational frequencies, along with many other properties are appreciable by this program (Joohari, 2015; Naghsh, 2018; Monajjemi, 2020; Dang, 2020).

Nuclear magnetic resonance (NMR) typically utilizes a tuned resonance circuit with impedance matching to transmit power and receive signal (Hopper, 2011; Le, 2020; Pham, 2020; Monajjemi, 2020). Parameters optimized in NMR including magnetic isotropic (σiso) and magnetic anisotropic (σaniso) shielding, $\sigma_{11,}\sigma_{22,}\sigma_{33}$, atomic charges, asymmetry parameter (η), chemical shift anisotropy (Δσ) and span (Ω) as shown in the following result for its fundamental importance in chemistry and biochemistry studies (Facelli, 2002), in which calculated in GIAO magnetic shielding for Dopamine and Serotonin by using B3LYP method with 6-31G(d) basis set which gathered in table 1-2.

Charge transfer and electrostatic potential-derived also calculated using the Merz-Kollman-Singh (MK) charge distribution scheme obtained from B3LYP/6-31G (Besler, 1984; Le, 2019; Monajjemi, 2019; Monajjemi, 2019) as it shown in table 4-5.

Quantum chemistry calculations have been fulfilled to determine the partial charges on atoms. For this purpose, the Merz-Kollman-Singh (MK) algorithm (Singh, 1984; Menegon, 2002; Bultinck, 2002; Monajjemi, 2019; Le, 2019) was used, because of the fact, that MK charges are derived from the electrostatic potential, they are known to be much less basis dependent in comparison with the Mulliken charges.

Frequency methods with uff/6-31 G basis set has also been assessed by zero-point energy correction, enthalpy, and Gibbs free energy presented in table 3. The ideas of quantum zero-point energy may be used to measure forces arising in electromagnetism, nuclear physics, and pair theory (HBoyer, 2011; Monajjemi, 2019; Pham, 2019; Pham, 2019; Pham, 2019).

3. RESULT AND DISCUSSIONR

In this work the NMR parameters as *Ab initio* calculation of nuclear magnetic shielding such as σ_{iso} (isotropy shielding) and σ_{aniso} (anisotropy shielding), asymmetry parameter (η), chemical shift anisotropy (Δσ) and span (Ω) for some of the carbon atoms in Dopamine and Serotonin-SWCNT complex have been theoretically studied. the magnetic properties of atomic nuclei and physical and chemical properties of atoms have shown in table 1-2.

According to table 1, in complex Dopamine+7.0 (nm) diameter SWCNT the most value of σiso belongs to $\mathbf{C_{111}}$ (132.6) and $\mathbf{C_1}$ has the most value of σaniso (431.1) and Ω (712.7), the most parameters of Δσ are positive and the maximum specified in $\mathbf{C_{25}}$(318.7) .$\mathbf{C_{54}}$ has the maximum amount of η (7.004), while The most content of etta (η) are negative.

For Dopamine+SWCNT (7.5 nm diameter) most positive results described below:
Maximum extent of σiso and σaniso shown in C_{54}(130.2) and C_1(188.05) and most values of Δσ, η and Ω respectively belong to C_{41}(180.4), C_{81}(1.46) and C_{15}(205.9). C_7 in Dopamine combined 7.7 (nm) SWCNT has the two-minimum value of σiso and σaniso and the maximum amount of these two parameters respectively specified for C_{81}(148.1) and C_{71} (165.4). Among positive values of Δσ and Ω, most value is for C_{23}(125.5) and for C_7(184.5) and C_1 has the most amount of η (5.3) and in the end of table 1, for medication connected to 10.0(nm)SWCNT C_{98} has the two maximum value of σiso and σaniso (2345.7 and 6599.9) and also C_7 has the two maximum value of Δσ and Ω (5109.2 and 10365.9) and minimum value of σiso (-3276.8). The Δσ parameter of NMR for carbon atoms in dopamine are shown in Fig.1.

Table 1. comparison of NMR chemical shielding tensors data calculated by B3LYP models with 6-31G (d) basis set for C atoms in Dopamine with 7.0,7.5,7.7,10.0 (nm)diameters SWCNT

Nanotube diameter	Atomic label	$\sigma_{Isotropic}$	$\sigma_{Anisotropy}$	$\Delta\sigma$	η	(Ω)
7.0(nm) diameter	C1	-61.9971	431.1205	125.94985	-2.669681754	712.7136
	C2	-55.9329	284.2069	-262.72185	-0.941227956	436.5767
	C7	70.2592	177.7319	-16.77315	-13.28529525	191.6289
	C23	51.2743	234.2899	231.56645	-0.203828102	258.2786
	C25	-28.7105	331.4964	318.79495	-0.108449211	378.3108
	C32	80.1372	255.5227	219.06665	0.225399262	327.8285
	C37	54.7445	245.1959	105.19445	0.247925152	201.8405
	C43	49.6047	268.2065	225.15495	-0.748621116	339.3801
	C54	56.7737	173.5293	9.6788	7.004473695	201.6148
	C57	56.1484	227.8706	-138.54925	-1.650464131	266.2388
	C65	62.4859	192.6591	-100.0975	-0.865877635	229.9987
	C71	60.3998	239.8636	-62.51745	-2.053075581	283.486
	C81	4.3217	287.7743	275.7912	-0.883150731	391.8035
	C92	11.918	230.2496	-61.76945	-0.224433943	287.0529
	C98	63.308	235.2389	-61.1212	-5.883482327	257.8256
	C105	8.0629	275.3461	202.95535	-0.711034296	320.4298
	C111	132.695	151.8513	-54.41835	3.382608072	172.0154
7.5 (nm) diameter	C1	120.137	188.0531	-57.725	-3.683176859	197.5842
	C7	128.2401	174.4124	-43.865	-2.9666	186.6264
	C15	111.4445	151.1551	107.48605	-1.15592163	206.9136
	C23	122.4577	183.9121	99.5384	0.51318	185.1918
	C25	128.9172	178.6165	119.7081	0.49403	187.0691
	C32	119.1856	187.3431	151.9811	-0.129	179.4674
	C36	128.868	160.761	118.141	0.162187556	167.3685
	C41	125.2164	182.8736	180.45925	-0.02099227	184.9352
	C43	127.3253	177.988	177.9551	0.22048	191.0786
	C54	130.2413	168.9081	90.9562	1.38125	190.2925
	C57	129.7138	172.4295	104.5858	0.57139	183.0504
	C65	126.7276	178.5838	-15.0607	-14.248	195.5395
	C72	130.9363	172.0715	-30.44975	-4.86461629	176.6094
	C81	120.7053	151.5337	115.9315	1.46449	200.2018
	C92	122.9333	175.8507	106.8202	0.43439	178.9967
	C105	127.371	153.9825	92.151	0.63219	183.2242
	C 125	126.3749	177.8	150.9622	0.55	182.91
7.7 (nm) diameter	C1	132.681	146.035	-19.37495	5.300645937	184.2307
	C4	132.6676	146.0568	129.92095	-0.04866998	184.3122
	C7	132.6689	145.9607	67.5803	-1.610657248	184.5438
	C15	145.6092	155.7815	-1.15065	52.35106244	163.5354
	C25	145.8312	155.7861	-82.42945	1.099072601	163.2435
	C32	146.5872	163.0894	-62.70495	1.13702746	169.048
	C37	146.6595	162.6306	35.988	-1.72453318	168.1706
	C43	146.4216	160.8268	11.8748	-5.0981406	170.6319
	C54	147.3921	160.0321	47.40945	-1.1672831	170.1198
	C57	147.859	163.9497	-72.37355	0.927175052	166.5406
	C60	147.9451	164.4014	-62.739	1.797666523	167.5336
	C65	148.6659	162.816	41.80385	-1.057312903	166.661
	C71	147.1292	165.4433	10.49405	-8.11758568	169.1089
	C81	148.1237	164.0148	-76.1874	1.058556927	167.1129
	C92	146.9118	157.0787	-59.56625	1.506931358	166.234
	C105	143.9076	161.8892	-54.40545	0.753313317	170.3449
	C 125	146.4518	155.0132	120.52035	0.009751465	163.0475
10.0 (nm) diameter	C1	-1388.4138	2479.4789	2250.5794	-2.875777125	4827.993
	C2	-1310.1002	2359.1903	2182.0785	-2.8750534	4602.4021
	C7	-3276.8369	5221.9061	5109.2273	-2.424260636	10365.904
	C23	-943.2285	1794.2354	1770.62155	-2.30857839	3436.1867
	C25	-1450.956	2556.5532	2403.2284	-2.411837277	4978.7921
	C32	585.6755	1286.1129	-684.24555	-2.516223671	1376.532
	C41	-168.6885	709.2541	302.01865	-3.17342803	1277.9586
	C43	-459.1714	1080.7943	1073.9781	-2.668578437	2087.1408
	C54	791.7969	1847.5768	-856.0683	-2.52629749	1921.9603
	C57	1042.8053	2604.2729	-1264.7287	-2.530554318	2679.8707
	C65	-362.4327	931.4973	759.3964	-2.697498915	1711.1428
	C71	1990.6444	7995.2979	-3678.92135	-1.79392268	8893.8852
	C81	-2438.9415	4738.534	3006.39335	-3.282596608	8949.3709
	C92	1530.8075	4238.4856	-1831.67415	-2.603544495	4280.0077
	C98	2345.7545	6599.9016	-3276.89115	-2.31090732	6613.7541
	C105	143.0013	103.6263	73.80605	1.63769409	134.4928
	C111	33.602	361.0106	158.48845	-1.765353416	599.3304

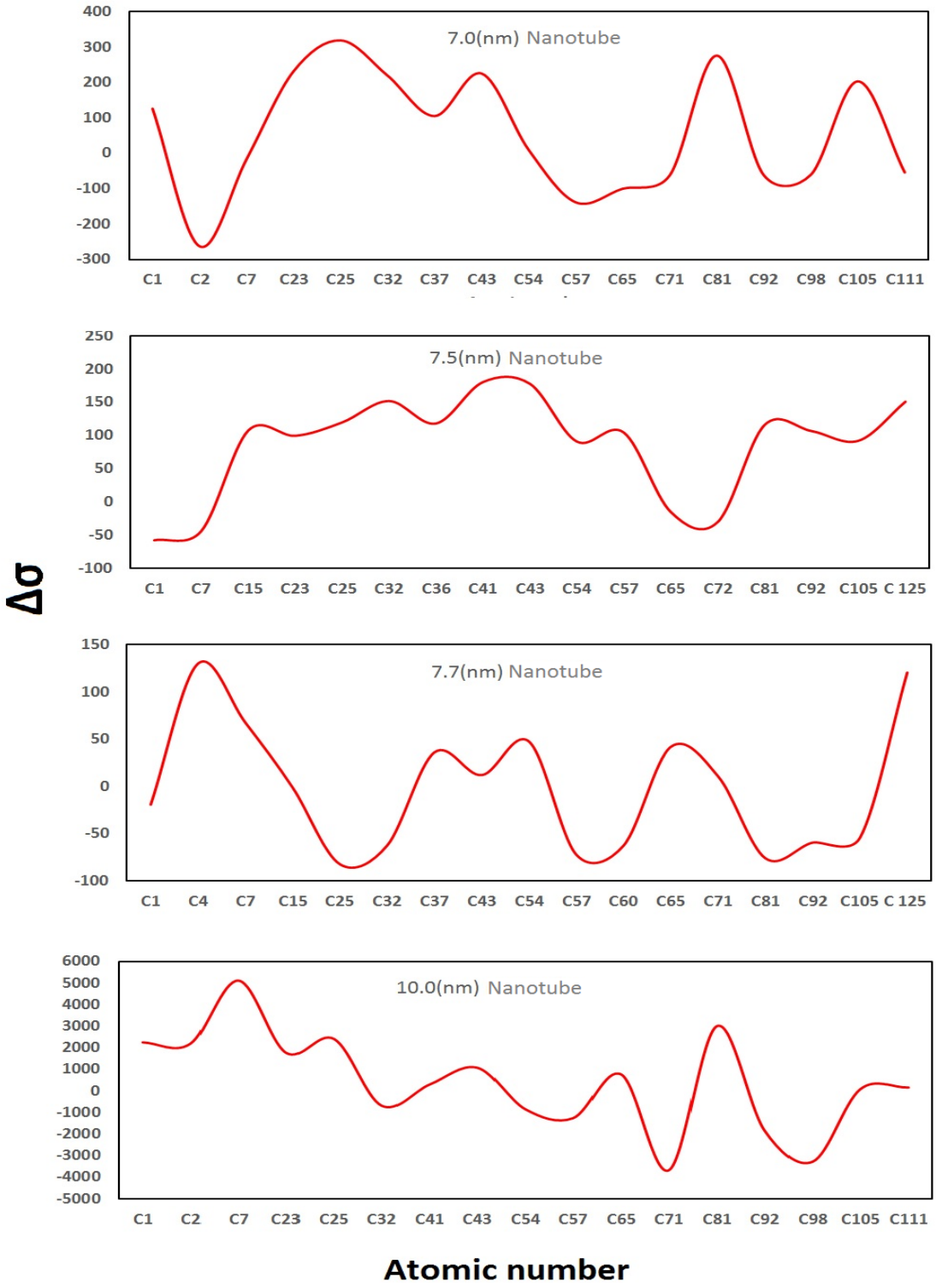

Fig. 1. Δσ parameter of NMR; calculated by B3LYP models with 6-31G (d) basis set for C atoms in Dopamine with 7.0,7.5,7.7,10.0 (nm)diameters SWCNT

Table 2. comparison of NMR chemical shielding tensors data calculated by B3LYP models with 6-31G (d) basis set for C atoms in Serotonin with 7.0,7.5,7.7,10.0 (nm)diameters SWCNT

Nanotube diameter	Atomic label	$\sigma_{Isotropic}$	$\sigma_{Anisotropy}$	$\Delta\sigma$	η	(Ω)
7.0(nm) diameter	C1	116.4332	140.9858	82.8902	-0.61646612	178.2112
	C7	74.2509	204.2218	-96.43575	-2.73489085	208.7471
	C8	71.6833	196.4182	-110.11735	-2.48652233	221.4184
	C13	6.6116	315.5116	-99.4292	-5.1722673	359.5881
	C25	28.3078	270.3146	250.47975	0.623975591	340.7136
	C32	12.9919	233.375	-76.9656	2.2632059	356.2582
	C39	73.6444	230.0081	205.44545	0.679074421	272.3334
	C43	51.3202	205.3721	-0.183834957	-86.1022316	-0.183834957
	C57	81.3243	177.24	-62.7376	-2.03901647	205.4642
	C65	58.7288	229.3421	-0.8894	42.39566	258.2022
	C78	-84.8294	533.0753	329.9972	0.029666615	878.1523
	C81	-5.0457	297.7524	290.15765	-0.83964235	381.2771
	C84	-2.4267	291.7623	169.5002	-0.18012191	362.0305
	C92	75.3088	233.9536	-72.7686	-3.17459041	261.0028
	C95	10.1508	273.4406	58.50525	0.897727127	322.9286
	C105	32.7953	289.2982	137.56345	0.507050746	352.6472
	C111	150.8713	94.6607	-27.1712	3.532291544	122.9843
7.5 (nm) diameter	C1	119.8483	188.1547	-59.097	-3.82773237	197.8378
	C7	123.3916	181.7667	-89.3649	-1.96540924	185.6545
	C14	124.8865	172.9518	-69.38185	-2.45907179	182.0775
	C25	129.2678	177.9716	-21.5596	-7.29479675	187.0531
	C27	122.8933	184.2623	63.47605	1.704753998	190.7664
	C32	129.0051	159.1898	65.06915	1.247598132	178.1161
	C43	127.7431	177.1281	104.26365	0.855883618	190.7271
	C49	109.5641	174.7717	174.25285	1.067521995	242.5449
	C57	128.8224	178.6361	178.5107	0.073214099	183.8459
	C59	125.6289	180.4202	156.14745	0.112632963	184.7249
	C65	122.0102	149.8532	28.2208	5.905293259	195.7234
	C70	123.4886	181.3623	140.2931	0.333615124	187.5683
	C81	120.5973	151.6663	28.05075	8.245816957	200.4143
	C87	129.566	171.6776	-18.73825	-9.78194602	185.9051
	C92	129.026	175.6672	-33.89155	-4.33780249	178.8916
	C105	126.1465	180.6666	-50.6156	-3.3504058	182.7211
	C125	126.0951	177.9827	176.30285	0.043463563	183.2879
7.7 (nm) diameter	C1	160.0612	104.76	-21.32715	-3.61506108	126.6316
	C7	135.3304	138.025	35.07945	-1.31414119	180.3636
	C15	148.1574	151.6621	6.21055	-4.50489087	158.9513
	C25	145.6633	156.1608	-82.45425	0.88012989	163.9731
	C27	145.5949	155.4306	152.84035	0.078529982	162.4718
	C32	146.6572	162.9422	-63.17045	1.587151113	169.0624
	C43	150.5976	153.8898	14.02605	-3.15836248	163.8515
	C51	146.212	161.7524	138.0016	-0.06204276	171.7281
	C57	149.9806	163.0474	-76.7552	1.16174409	167.4272
	C60	148.4412	164.0148	-61.9224	0.960626526	166.9198
	C65	147.0628	165.6413	39.7976	-0.94253171	167.4507
	C81	148.0398	164.5705	-75.8767	1.309603607	167.5875
	C92	146.5586	161.5587	-65.5776	1.027086993	169.8241
	C99	146.7288	162.3846	2.89865	-23.8520518	168.7669
	C105	146.6955	163.0194	-66.23605	1.453032752	168.4526
	C106	146.5392	163.5071	-57.88785	1.397715583	168.953
	C125	145.583	156.0022	122.8915	-0.0398034	163.6274
10.0 (nm) diameter	C1	19.582	235.182	-111.68145	-1.76457908	283.3032
	C4	521.7316	1059.7161	-473.89885	-3.2537244	1096.9219
	C7	870.3555	2098.6893	-1075.0815	-2.82456744	2136.5468
	C8	630.2476	1385.0651	-653.74295	-3.07860291	1417.3609
	C14	227.4063	219.4072	-18.5734	-15.2379694	275.3438
	C25	422.5754	734.9325	-425.0484	-2.36265305	805.3255
	C32	133.2455	196.3262	130.8842	0.9977	-177.462464
	C43	263.358	257.8087	-53.5824	-8.09252665	330.6118
	C57	-31.7412	426.6604	327.10215	-2.68408768	695.9907
	C65	251.2293	230.0311	-183.1533	-1.49321798	304.3239
	C69	247.0161	218.8922	-40.4807	-9.77402812	294.7551
	C73	-104.0341	534.4774	494.7451	-2.33363504	911.4645
	C81	178.5111	102.888	-114.6782	0.740612427	147.1954
	C92	-269.4006	722.5244	661.7302	-3.02345034	1372.9567
	C94	-485.1518	1031.7152	1005.4664	-2.78605809	1990.3419
	C105	156.9733	89.7987	71.9148	0.848958768	118.8076
	C111	152.9726	106.1711	81.5342	-0.63634769	130.6261

As it shown in table 2, in Serotonin +7.0 (nm) SWCNT complex, C_1 has the most value of σiso (116.4) and the most value of σaniso, Δσ and Ω demonstrated in C_{78} which respectively equals with 533.07,329.9 and 787.1 and C_{65} has the most value of η (42.3). In Serotonin+7.5 nm diameter SWCNT complex, the maximum level of σiso and σaniso respectively belongs to C_{87}(129.5) and C_1(188.1) and the minimum level belongs to C_{49}(109.5) and C_{65}(149.8) and also the maximum level of Δσ and Ω are respectively 187.5 and 242.5 which belongs to C_{57} and C_{42}. Most of the etta (η) parameters have been reported positive and the maximum value belongs to C_{81} (8.2). C_1 in drug+7.7(nm)diameter SWCNT has the two maximum and minimum value of σiso (160.01) and σaniso (104.7) and the minimum value of σiso (135.3) and maximum value of Ω (242.5) also belongs to C_7. As it specified in these results, the most value of σaniso, Δσ and η are for C_{65}(165.6), C_{27}(152.8) and C_{32}(1.58). C_7 in Serotonin connected to SWCNT (10.0nm diameter) has the most value of σiso (870.3) , σaniso(2098.6) and Ω(2136.5) . Most of the Δσ and etta (η) parameters have been reported negative and the maximum values belong to C_{94} (1005.4) and C_{32}(0.9). The η parameter of NMR for carbon atoms in serotonin are shown in Fig.2.

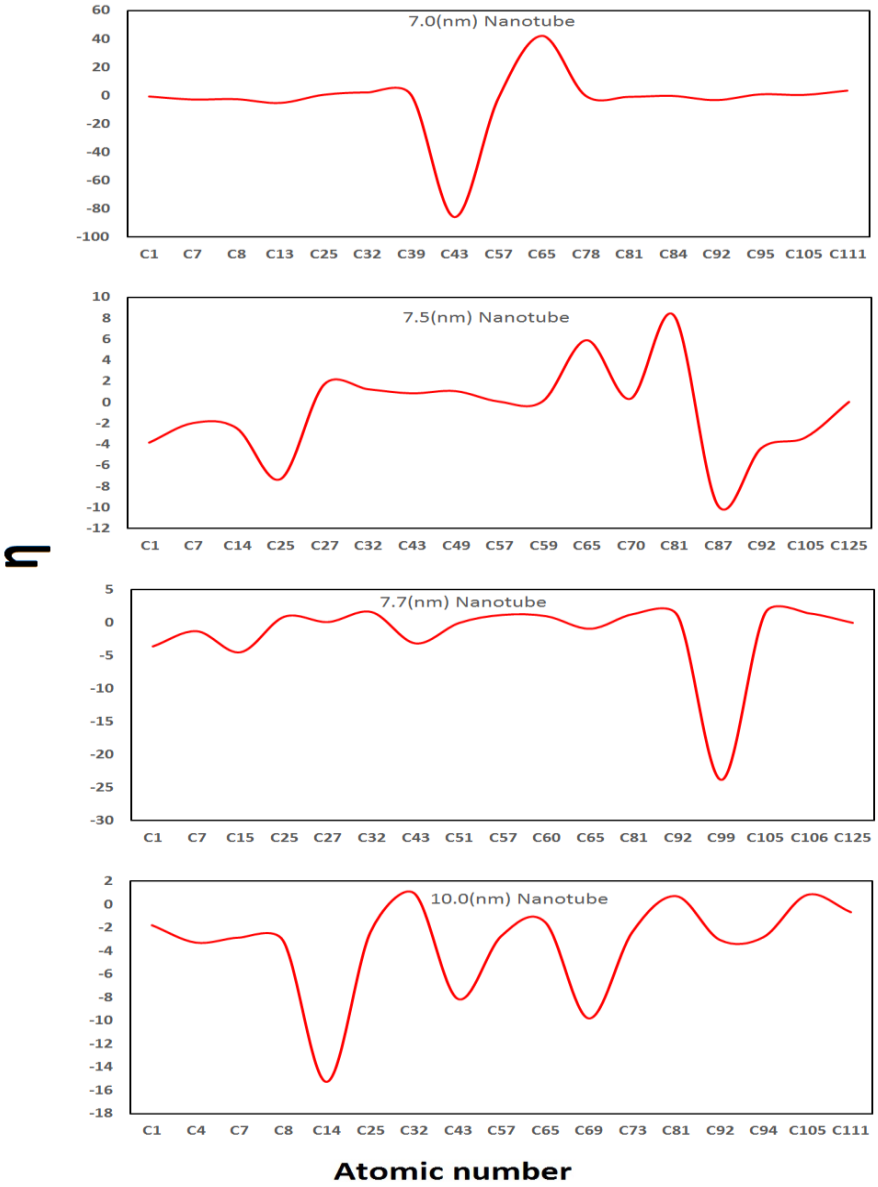

Fig.2. η parameter of NMR; calculated by B3LYP models with 6-31G (d) basis set for C atoms in Serotonin with 7.0,7.5,7.7,10.0 (nm)diameters SWCNT

Thermodynamic paraeters including zero-point energy, total energy, enthalpies (ΔH) and Gibbs free energy (ΔG) of the complex were computed by Freq method using Uff/6-31G(d) obtained and summarized in table3. Also, we can comparison atom charge distributions in MK method for the two-molecule complex in table 4-5.

Table 3. Zero-point energy, total correction energy, enthalpy and free gibs energy analysis of B3LYP method in uff/6-31G basis set

	7,0-dopamine	7,0-serotonin	7,5-dopamine	7,5-serotonin	7,7-dopamine	7,7-serotonin	10,0-dopamine	10,0-serotonin
E_{ZPE}	1.134665	1.164751	1.772866	1.804665	1.737421	1.774504	1.296485	1.329319
E_{tot}	1.186675	1.216071	1.830497	1.863011	1.787204	1.823544	1.331974	1.364415
H_{corr}	1.187619	1.217015	1.831441	1.863955	1.788148	1.824488	1.332918	1.365359
G_{corr}	1.062814	1.096034	1.698319	1.729044	1.663745	1.703395	1.236122	1.270746
$E_0 = \varepsilon_0 + E_{ZPE}$	4.044015	4.050447	5.691152	7.530773	4.684883	4.841821	3.870821	3.950483
$E = \varepsilon_0 + E_{tot}$	4.096024	4.101766	5.748783	7.589119	4.734665	4.89086	3.90631	3.985579
$H = \varepsilon_0 + H_{corr}$	4.096968	4.102711	5.749727	7.590063	4.735609	4.891804	3.907254	3.986523
$G = \varepsilon_0 + G_{corr}$	3.972163	3.98173	5.616606	7.455152	4.611206	4.770712	3.810458	3.89191

Table4.Merz-Kollman parameters analyses of Dopamine+SWCNT carbon atoms in BLYP3/3-61(d) level of theory

Dopamine +7.0 nm SWCNT				Dopamine +7.5 nm SWCNT			
Atomic label	ΔV=(V2-V1)	Δq	ΔV=(k(q2-q1)/R21)	Atomic label	ΔV=(V2-V1)	Δq	ΔV=(k(q2-q1)/R21)
Atom92-Atom 2	-0.02807	0.131906	4.68363E+18	Atom 41-Atom 25	-0.000616	0.002743	1.75796E+17
Atom76-Atom62	-0.022281	0.021203	7.48639E+17	Atom 111-Atom 45	0.005974	0.000326	3.64132E+15
Atom90-Atom88	-0.005501	-0.006014	-3.56063E+17	Atom 72-Atom 56	-0.002334	-0.003544	-2.26055E+17
Atom71-Atom54	0.010647	-0.011558	-3.7709E+17	Atom 118-Atom 53	0.002178	0.000472	5.17041E+15
Atom86-Atom70	0.006281	-0.022734	-1.51919E+18	Atom 63-Atom 62	0.000793	0.001372	8.75176E+16
Atom37-Atom35	0.014977	0.139343	8.25474E+18	Atom 102-Atom 70	0.001731	-0.000655	-1.01306E+16
Atom98-Atom23	-0.004162	-0.147796	-2.89676E+18	Atom 148-Atom 22	-0.005766	-0.003312	-1.23162E+17
Atom79-Atom77	-0.007455	-0.065044	-3.82505E+18	Atom 131-Atom 36	0.004748	0.011702	1.42561E+17
Atom81-Atom37	-0.003872	-0.084847	-1.27372E+18	Atom 61-Atom 46	0.002981	0.001505	9.59932E+16
Atom87-Atom85	-0.01285	0.003761	2.20294E+17	Atom 32-Atom15	-0.00244	0.003913	2.49531E+17
Dopamine +7.7 nm SWCNT				Dopamine +10.0 nm SWCNT			
Atomic label	ΔV=(V2-V1)	Δq	ΔV=(k(q2-q1)/R21)	Atomic label	ΔV=(V2-V1)	Δq	ΔV=(k(q2-q1)/R21)
Atom100-Atom94	0.00108	0.001508	1.00785E+17	Atom 52-Atom 50	-0.00021	-0.002201	-3.87102E+16
Atom 38-Atom31	0.000015	-0.000244	-1.62382E+16	Atom 39-Atom 23	0.001707	-0.001737	-2.18651E+16
Atom 86-Atom79	0.000709	0.000327	2.18433E+16	Atom 29-Atom 19	0.000105	0.015327	1.02405E+18
Atom 37-Atom15	-0.000669	0.008765	5.84167E+17	Atom 78-Atom 67	-0.001047	-0.001899	-1.26797E+17
Atom 60-Atom53	-0.00013	0.000213	1.42459E+16	Atom 71-Atom 70	-0.004524	-0.003461	-2.31075E+17
Atom 121-Atom 114	-0.001012	-0.002792	-1.85095E+17	Atom 20-Atom 1	0.01917	0.047153	3.14007E+18
Atom 136-Atom 115	-0.016153	-0.061738	-4.12166E+18	Atom 38-Atom 24	0.001128	-0.001435	-1.98419E+16
Atom 25-Atom4	0.016365	0.061404	4.09939E+18	Atom 90-Atom 80	0.000146	-0.017473	-1.16614E+18
Atom 95-Atom88	-0.000061	-0.000062	-4.14516E+15	Atom 98-Atom 93	-0.002693	-0.001574	-2.07089E+16
Atom 134-Atom 127	-0.003173	-0.007945	-5.32255E+17	Atom 60-Atom 41	0.001456	0.001554	1.03684E+17

Zero-point energy (E_{ZPE}), total correction energy (E_{TOT}), enthalpy (H_{corr}) and free gibs energy (G_{corr}) value demonstrated in table3, as it shown below the most value of these parameters specified for Dopammine+7.5(nm) SWCNT and for Serotonin+7.5 (nm) SWCNT and respectively are equal with:

$E_{ZPE\ (Dopamine)}$: 1.77 $E_{ZPE\ (Serotonin)}$: 1.8
$E_{TOT\ (Dopamine)}$:1.83 $E_{TOT(Serotonin)}$:1.86
$H_{corr\ (Dopamine)}$:1.83 $H_{corr\ (Serotonin)}$:1.86
$G_{corr\ (Dopamine)}$:1.69 $G_{corr\ (Serotonin)}$:1.72

Potential difference energy and atomic charge energy of Dopamine and Serotonin complex listed in table 4-5 and according to the table 4, in Dopamine connected to SWCNT (7.0 nm diameter) complex C_{37}-C_{35} has the most value of ΔV (0.014) and C_{98}-C_{23} has the most value of Δq (-0.014).In Dopamine connected to SWCNT (7.5 nm diameter) complex C_{131}-C_{36} has the most value of ΔV (0.004) and C_{72}-C_{56} has the most value of Δq (-0.003).For Dopamine connected to SWCNT (7.7 nm diameter) complex C_{25}-C_4 has the most value of ΔV (0.016) and C_{136}-C_{15} has the most value of Δq (-0.06) and In Dopamine connected to SWCNT (10.0 nm diameter) complex C_{20}-C_1 has the most value of ΔV (0.019) and C_{90}-C_{80} has the most value of Δq (-0.017).

Based on table 5 ,in Serotonin connected to SWCNT (7.0 nm diameter) complex C_{84}-C_{38} has the most value of ΔV (0.02) and C_{101}-C_{85} has the most value of Δq (-0.04).In Serotonin connected to SWCNT (7.5 nm diameter) complex C_{125}-C_{44} has the most value of ΔV (0.15) and C_{33}-C_{31} has the most value of Δq (-0.07).For Serotonin connected to SWCNT (7.7 nm diameter) complex C_{17}-C_{11} has the most value of ΔV (0.015) and C_{114}-C_{107} has the most value of Δq (-0.01) and In Serotonin connected to SWCNT (10.0 nm diameter) complex C_{54}-C_{48} has the most value of ΔV (29.0) and C_{94}-C_{84} has the most value of Δq (-0.047).

Table5.Merz-Kollman parameters analyses of Serotonin +SWCNT carbon atoms in BLYP3/3-61(d) level of theory

Serotonin +7.0 nm SWCNT				Serotonin +7.5 nm SWCNT			
Atomic label	ΔV=(V2-V1)	Δq	ΔV=(k(q2-q1)/R21)	Atomic label	ΔV=(V2-V1)	Δq	ΔV=(k(q2-q1)/R21)
Atom95-Atom 79	0.020936	0.023892	1.4059E+18	Atom 59-Atom 44	0.00212	0.072666	4.65404E+18
Atom 84-Atom 38	0.027323	0.003392	6.02589E+16	Atom 70-Atom 69	0.00064	0.000821	5.23539E+16
Atom 78-Atom 62	0.008191	0.003824	2.25269E+17	Atom 137-Atom 43	0.008244	0.001325	1.69242E+16
Atom 101-Atom 85	-0.014437	-0.041175	-2.45136E+18	Atom 33-Atom 31	-0.039698	-0.071583	-4.56231E+18
Atom 105-Atom 103	-0.003069	0.019313	1.14173E+18	Atom 43-Atom 27	-0.000042	-0.001991	-1.26979E+17
Atom 41-Atom 39	-0.003487	0.01977	1.17218E+18	Atom 51-Atom 36	0.002899	0.01377	8.82197E+17
Atom 78-Atom 33	-0.003959	-0.003122	-5.09644E+16	Atom 87-Atom 71	-0.002846	-0.003596	-2.2931E+17
Atom 102-Atom 13	-0.000746	0.016571	9.82742E+17	Atom 125-Atom 44	0.015214	0.002927	3.20581E+16
Atom 24-Atom 8	0.014363	0.016136	9.53403E+17	Atom 16-Atom 14	0.003046	-0.000785	-5.00443E+16
Atom 55-Atom 43	-0.00887	0.012785	7.56531E+17	Atom 112-Atom 49	-0.002538	0.068997	7.63021E+17
Serotonin +7.7 nm SWCNT				Serotonin +10.0 nm SWCNT			
Atomic label	ΔV=(V2-V1)	Δq	ΔV=(k(q2-q1)/R21)	Atomic label	ΔV=(V2-V1)	Δq	ΔV=(k(q2-q1)/R21)
Atom37-Atom 15	-0.002547	0.013943	9.28641E+17	Atom 64-Atom 54	-29.093429	-0.000513	-3.4306E+16
Atom 58-Atom 51	-0.001182	-0.000613	-4.09662E+16	Atom 24-Atom 14	-0.001222	0.012735	8.5139E+17
Atom 108-Atom 101	-0.000326	-0.00021	-1.3975E+16	Atom 54-Atom 48	29.09457	0.00107	1.4844E+16
Atom 17-Atom 11	0.015898	0.061568	4.11071E+18	Atom 94-Atom 84	-0.019428	-0.047381	-3.15734E+18
Atom 106-Atom 99	0.000272	0.000334	2.22229E+16	Atom 69-Atom 52	-0.001998	-0.001771	-2.65049E+16
Atom 80-Atom 73	-0.000132	0.000182	1.21748E+16	Atom 36-Atom 25	0.002073	0.002912	1.94438E+17
Atom 27-Atom 16	0.001942	0.000847	8.47164E+15	Atom 8-Atom 4	-0.001528	-0.00115	-1.52978E+16
Atom 114-Atom 107	0.00326	-0.010612	-7.0728E+17	Atom 32-Atom 31	0.0091	0.017025	6.73366E+17
Atom 81-Atom 60	-0.000004	0.00007	4.68155E+15	Atom 62-Atom 51	-0.000238	-0.002146	-7.28257E+16
Atom 29-Atom 22	-0.014864	-0.014207	-9.50012E+17	Atom 89-Atom 73	-0.005511	-0.017111	-2.17137E+17

4.CONCLUSION

In this work, we theoretically investigated the structure features of Dopamine and Serotonin as a biological active compound and single-walled carbon nanotube as a biological transfer. Chemical shift anisotropy asymmetry (η), isotropy (σ iso), anisotropy (σ aniso), $\Delta\sigma$, K and chemical shift tensor (δ) were calculated based on theoretical data obtained from BL3Y/6-31G(d) levels of theory. Moreover, thermodynamic analyses with uff/6-31 G basis set were performed and then stabilization energies such as Zero-point energy, total correction, enthalpy and free Gibs energy and also Merz-Kollman Singh (MK) analysis carried out by gaussian 09 application.

5. REFERENCES

Berger, M.; Gray, J.A.; Roth, B.L. (2009) The expanded biology of serotonin. *Annu Rev Med*, 60, 355–66. doi: 10.1146/annurev.med.60.042307.110802.

Berridge, K.C.; Robinson, T.E.; Aldridge, J.W. (2009) Dissecting components of reward: 'liking', 'wanting', and learning. *Current Opinion in Pharmacology*, 9, 65–73. doi:10.1016/j.coph.2008.12.014. PMC 2756052. PMID 19162544.

Besler, B.H.; Merz, K.M.; Kollman P.A. (1990) Atomic Charges Derived from Semiempirical Methods, J. comp. Chem.,11 ,431-439.

Boyer, H.T. (1970) Quantum zero-point energy and long-range forces, Annals of physics, 56, 474-503. Doi: 10.1016/0003-4916(70)90027-8

Brami-Cherrier, K.; Valjent, E.; Garcia, M.; Pages, C.; Hipskind, R.A.; Caboche, J. (2002) Dopamine induces a PI3-kinase-independent activation of Akt in striatal neurons: a new route to cAMP response elementbinding protein phosphorylation. *Journal of Neurosci*, 22, 8911–8921

Bultinck, P.; Langenaeker, W.; Lahorte, P.; Proft, F.D.; Geerlings, P.; Alsenoy, C.V.; Tollenaere, J.P. (2002) The Electronegativity Equalization Method II: Applicability of Different Atomic Charge Schemes, *J Phys Chem A*, 106, 7895-7908.

Conn, P.J.; Sanders-Bush, E. (1984) Selective 5-HTe antagonists inhibit serotonin stimulated phosphatidylinositol metabolism in cerebral cortex, *Neuropharmacology*, 23, 993-996.

Conn, P.J.; Sanders-Bush, E. (1986) Agonist-induced phosphoinositide hydrolysis in choroid plexus, *J. Neurochem.*, 47, 1754–1760.

Dang, D.M.T.; Monajjemi, M.; Mollaamin, F.; Dang, C.M. (2020) Simulation of droplet ejection based on electromechanical parameters & chemical condition for controlling inkjet printing devices Biointerface Research in Applied chemistry, 10, 5361–5368. https://doi.org/10.33263/BRIAC103.361368

Deutch, A.Y.; Roth, R.H.; (1999) Neurotransmitters. In Fundamental Neuroscience, *Academic Press* 193–234,

Dickson, D.V. (2007) Neuropathology of movement disorders, In Tolosa E, Jankovic JJ (eds.). Parkinson's disease and movement disorders. Hagerstown, MD: Lippincott Williams & Wilkins, 271–83. ISBN 978-0-7817-7881-7.

Endo, Y.; Shibazaki, M.; Nakamura, M.; Takada, H. (1997) Contrasting effects of lipopolysaccharides (endotoxins) from oral black-pigmented bacteria and Enterobacteriaceae on platelets, a major source of serotonin, and on histamine-forming enzyme in mice, *J Infect Dis***,** 175, 1404–12. doi:10.1086/516473

Facelli, J.C. (2002) Encyclopedia of Nuclear Magnetic Resonance; D. M. Grant, R. K. Harris, Eds., London: John Wiley & Sons., 9, 323.

Herr, N.; Bode, C.; Duerschmied, D. (2017) The effects of Serotonin in immune Cells, *Front. Cardiovasc. Med*, 20, 48. doi.org/10.3389/fcvm.2017.00048.

Hopper, T.; Mandal, S.; David, C.; Hürlimann, M.; Yi-Qiao, S. (2011) Low-frequency NMR with a non-resonant circuit, *Journal of Magnetic Resonance*, 210, 69-74. Doi: 10.1016/j.jmr.2011.02.014

Howes, O.D; Kapur, S. (2009) The dopamine hypothesis of schizophrenia: version III—the final common pathway, *Schizophrenia Bulletin*, 35, 549–62. doi:10.1093/schbul/sbp006. PMC 2669582. PMID 19325164.

Hoyer, D. (1988) Molecular pharmacology and biology of 5-HT 1 C receptors, *Trends Pharmacol. Sci.,* 9, 89-94.

Joohari, S.; Monajjemi, M. (2015) NMR and NBO study of vinblastine as a biological inhibitor.; Bulgarian Chemical Communications, 47, 631-646.

Julius, D.; MacDermott, A.B.; Axel, R.; Jesse, T. (1988) Molecular characterization of a functional cDNA encoding the serotonin lc receptor, *Science,* 241, 558–564
Kienast, T.; Heinz, A. (2006) Dopamine and the diseased brain. *CNS Neurol Disord Drug Targets*, 5, 109–31.

Le, C.M.T.; Mollaamin, F.; Dang, D.M.T.; Monajjemi, M.; Dang, C.M. (2019) Realistic simulation of the polymers in inkjet process: the investigation of physical phenomena in the ejection of a droplet, Biointerface Research in Applied chemistry, 9, 3949–3955. https://doi.org/10.33263/BRIAC93.949955

Le, C.M.T.; Monajjemi, M.; Pham, T.T.; Mollaamin, F.; Dang, C.M. (2020) Diffusion & concentration effect of Li/Li+ to the efficiency of LIBs, *Biointerface Research in Applied chemistry*, 10, 5076–5084. https://doi.org/10.33263/BRIAC102.076084

Le, C.M.T.; Monajjemi, M.; Pham, T.T.; Mollaamin, F.; Dang, C.M. (2019), Simulation & modelling of dilute solutions in drop-on-demand inkjet printing: a review, *Biointerface Research in Applied chemistry*, 9, 4474 – 4484, https://doi.org/10.33263/BRIAC96.474484

Lindemann. L.; Hoener, M.C. (2005) A renaissance in trace amines inspired by a novel GPCR family, *Trends Pharmacol. Sci.* 26, 274–281. doi:10.1016/j.tips.2005.03.007. PMID 15860375

Menegon, G.; Shimizu, K.; Farah, J.P.S.; Dias, L.G.; Chaimovich, H. (2002) Parameterization of the electronegativity equalization method based on the charge model 1, *Phys Chem Chem Phys*, 4, 5933-5936.

Miller, G.M. (2011) The emerging role of trace amine-associated receptor 1 in the functional regulation of monoamine transporters and dopaminergic activity, *Journal of Neurochemistry*, 116, 164–76. doi:10.1111/j.1471-4159.2010.07109.x. PMC 3005101. PMID 21073468 https://draxe.com/health/dopamine/

Mollaamin, F.; Pham, T.T.; Dang, D.M.T.; Monajjemi, M.; Dang, C.M. (2019) Modelling and Controlling of ion transport rate efficiency in Proton exchange membrane (PEMFC), alkaline (AFC), direct methanol

(DMFC), phosphoric acid (PAFC), direct forming acid(DFAFC) and direct carbon (DCFC) fuel cells, *Biointerface Research in Applied chemistry*, 9, 4050-4059. https://doi.org/10.33263/BRIAC94.050059

Monajjemi, M. (2019), Artificial intelligence & self-consistent sonification method for converting DNA sequence to music, *Biointerface Research in Applied chemistry*, 9, 4494–4501, https://doi.org/10.33263/BRIAC96.494501

Monajjemi, M. (2019) C-NMR sonification of human insulin: a method for conversion of amino-acid sequences to music notes, *Biointerface Research in Applied chemistry*, 9, 4077–4084. https://doi.org/10.33263/BRIAC94.077084

Monajjemi, M. (2019) Molecular vibration of dopamine neurotransmitter: a relation between its normal modes and harmonic notes, *Biointerface Research in Applied chemistry*, 9, 3956–3962. https://doi.org/10.33263/BRIAC93.956962

Monajjemi, M., (2019) Molecular biology's symphony orchestra from DNA to ribosome: a sonification from gene to protein, *Biointerface Research in Applied chemistry*, 10, 5679–5688. https://doi.org/10.33263/BRIAC104.679688

Monajjemi, M.; Mollaamin, F.; Shojaei, S. (2020) An overview on Coronaviruses family from past to Covid-19: introduce some inhibitors as antiviruses from Gillan's plants, *Biointerface Research in Applied chemistry*, 10, 5575–5585. https://doi.org/10.33263/BRIAC103.575585

Monajjemi, M.; Naghsh, F.; Mollaamin, F. (2020) Bio-Lipid Nano Capacitors: Resonance with Helical Myeline Proteins, *Biointerface Research in Applied chemistry*, 10, 6695–6705. https://doi.org/10.33263/BRIAC106.66956705

Monajjemi, M.; Mollaamin, F. (2020) Bio-capacitor consist of insulated myelin-sheath and uninsulated node of Ranvier: a bionano-antenna, *Biointerface Research in Applied chemistry*, 10, 4956–4965. https://doi.org/10.33263/BRIAC101.956965

Monajjemi, M.; Shahriari, S.; Mollaamin, F. (2020) Evaluation of Coronavirus Families & Covid-19 Proteins: Molecular Modeling Study, *Biointerface Research in Applied chemistry*, 10, 6039–6057. https://doi.org/10.33263/BRIAC105.60396057

Mössner, R.; Lesch, K.P. (1998) Role of serotonin in the immune system and in neuroimmune interactions, *Brain Behav Immun*, 12, 249–71. doi:10.1006/ brbi.1998.0532

Naghsh, F.; Monajjemi, M.; Zare, K. (2018) A conceptual model of microtubules as a macrobiological molecule and Quantum Consciousness, *Biointerface Research in Applied chemistry*, 8, 3758 – 3763.

Pantarotto, D.; Singh, R.; McCarthy, D.; Erhardt, M.; Briand, J.P.; Prato, M. et al. (2004). Functionalized carbon nanotubes for plasmid DNA gene delivery, Angew. *Chem. Int. Ed.*, 43, 5242–5246. doi: 10.1002/anie.200460437

Peroutka, S.J. (1990) 5-Hydroxytryptamine receptor subtypes, *Pharmacol. Toxicol*., 67, 373–383.

Pham, T.T.; Monajjemi, M.; Dang, D.M.T.; Mollaamin, F.; Dang, C.M. (2019) Reaction of cell membrane bilayers "as a variable capacitor" with G-protein: a reason for neurotransmitter signaling, *Biointerface Research in Applied chemistry*, 9, 3874–3883. https://doi.org/10.33263/BRIAC92.874883

Pham, T.T.; Monajjemi, M.; Dang, D.M.T.; Mollaamin, F.; Dang, C.M. (2019) Nano-capacitors as batteries including graphene electrodes and Ga-N mixed with biopolymers as insulator, *Biointerface Research in Applied chemistry*, 9, 3806–3811. https://doi.org/10.33263/BRIAC91.806811

Pham, T.T.; Monajjemi, M.; Dang, D.M.T.; Mollaamin, F.; Khakpour, A.; Dang, C.M. (2019) An overview of bio-interface electrolyte and Li2FePO4F as cathode in Li-ion batteries, *Biointerface Research in Applied chemistry*, 9, 3866 – 3873. https://doi.org/10.33263/BRIAC92.866873

Pham, T.T.; Monajjemi, M.; Mollaamin, F.; Dang, C.M. (2020) Advanced materials for family of fuel cells: a review of polymer electrolyte membrane, *Biointerface Research in Applied chemistry*, 10, 4853 – 4863. https://doi.org/10.33263/BRIAC101.853863

Reed, A.E.; Curtiss, L.A.; Weinhold, F. (1988) Intermolecular Interactions from a Natural Bond Orbital, Donor-Acceptor Viewpoint, *Chem. Rev*., 88, 899-926.

Robinson, T.E.; Berridge, K.C. (1993) The neural basis of drug craving: an incentive-sensitization theory of addiction, *Brain Research. Brain Research Reviews*, 18, 247–91. doi:10.1016/0165-0173(93)90013-p. PMID 8401595

Romanelli, R.J.; Williams, J.T.; Neve, K.A. (2009) Chapter 6: Dopamine receptor signalling: intracellular pathways to behavior, In Neve KA (ed.). The Dopamine Receptors. *Springer*. 137–74. ISBN 978-1-60327-333-6.

Singh, U.C.; Kollman, P.A. (1984) An approach to computing electrostatic charges for molecules, *J Comput Chem*, 5, 129-145.

Tîlmaciu, C.M.; May C.; Morris, M.C. (2015) Carbon nanotube biosensors; *Frontiers in Chemistry*, 3, 1-21. doi:10.3389/fchem.2015.00059

Vanderschuren, L.J.; Kalivas, P.W. (2000) Alterations in dopaminergic and glutamatergic transmission in the induction and expression of behavioral sensitization: a critical review of preclinical studies. *Psychopharmacol Ber,l* 151, 99–120.

Wagner, D.D.; Frenette, P.S. (2008) The vessel wall and its interactions, *Blood*, 111, 5271–81. doi:10.1182/blood-2008-01-078204
Wang, X. et al. (2019) The Prospective Value of Dopamine Receptors on Bio-Behavior of Tumor, *Journal of Cancer*, 10, 1622–1632. doi:10.7150/jca.27780.PMCID.PMC6548012

Wise, R.A. (2004) Dopamine, Learning and Motivation, *Nature reviews Neuroscience*, 5, 483-494. doi:10.1038/nrn1406

Xiangdang, S.; McGinty, J.F. (2010) D1 and D2 dopamine receptors differentially mediate the activation of phosphoproteins in the striatum of amphetamine-sensitized rats, *Psychopharmacology*, 214, 653-63. DOI 10.1007/s00213-010-2068-4.

Yu, B.; Becnel, J.; Zerfaoui, M.; Rohatgi, R.; Boulares, A.H.; Nichols, C.D. (2008) Serotonin 5-hydroxytryptamine(2A) receptor activation suppresses tumor necrosis factor-alpha-induced inflammation with extraordinary potency, *J Pharmacol Exp Ther*, 327, 316–23. doi:10.1124/jpet.108.143461

Zhu, H.W.; Xu, C.L.; Wu, D.H.; Wei, B.Q.; Vajtai, R.; Ajayan, P. M. (2002) Direct synthesis of long single-walled carbon nanotube strands, *Science*, 296, 884–886. doi: 10.1126/science.1066996.