Int. J. Electrochem. Sci., 5 **(2010)** 355 - 366

International Journal of ELECTROCHEMICAL SCIENCE
www.electrochemsci.org

Electronic and Geometry Studies on Swainsonine, DNA Base Pairs and its Complex

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Received: 24 February 2010 / *Accepted:* 15 March 2010 / *Published:* 31 March 2010

This research is designed to further understand the physicochemical interaction between the novel drug SW, and its biological receptor DNA. The ultimate goal is to design drugs that interact more with DNA. Understanding the physicochemical properties of the drug as well as the mechanism by which it interacts with DNA should ultimately enable the rational design of novel anti-cancer or anti-viral drugs. Molecular modeling on the complex formed between SW and DNA presented this complex to be fully capable of participating in the formation of a stable intercalation site. Furthermore, the molecular geometries of SW and DNA bases (Adenine, Guanine, Cytosine and Thymine) were optimized with the aid of the B3LYP/6-31G* method. The properties of the isolated intercalator and its stacking interactions with adenine···thymine (AT) and guanine···cytosine (GC) nucleic acid base pairs were studied with the DFTB method, an approximate version of the DFT method that was extended to cover the London dispersion energy. The B3LYP/6-31G* stabilization energies of the intercalator···base pair complexes were found to be -43.92 kcal/mol and -50.20 for AT···SW and GC···SW, respectively. It was concluded that dispersion energy and the electrostatic interaction contributed to stability of the intercalator·DNA base pair complexes. Results from comparison of the DFTB method and HF method conclude close results and support each other.

Keywords: DNA, Intercalator, Swainsonine, Chemometrics, DFTB, Drug Design, Base pairs

1. INTRODUCTION

Swainsonine, an a-mannosidase inhibitor which blocks Golgi oligosaccharide processing, represents a new class of compounds that inhibit both rate of tumor growth, and metastasis, in murine experimental tumor models [1]. In addition, swainsonine, an indolizidine alkaloid, is a potent inhibitor of lysosomal a-mannosidase and perhaps other mannosidases [2]. The unique ability of swainsonine to

exhibit antimetastatic, antiproliferative, and immunomodulatory activity imparts this drug a promising future in cancer therapy [3].

In recent years the DFT method was applied in different branches of chemistry [4-38]. This paper presents the recently introduced approximate DFT method, DFTB technique (density functional tight-binding), empirical London dispersion energy term, which is accurate and reliable for computational studies [39,40], and calculations performed using the DFTB technique for H-bonded and stacked DNA base pairs [41,42]. Furthermore, this computationally very efficient procedure can yet be used in quantum mechanical (QM) and QM/molecular mechanical (MM) MD simulations very conveniently and accurately [43,44].

The quantum mechanical description of interactions between SW and DNA base pairs (*Watson-Crick base pairing*) employing the DFTB method are reported in this paper. To achieve this goal SW and DNA base pairs were simulated and; atomic charges, geometrical values (bond lengths, bond angles and dihedral angles), dipole moment, polarizability, and energies of the frontier molecular orbitals (HOMO and LUMO) were obtained. According to a literature survey, this is the first paper that studies SW and DNA base pair intercalations using the DFT method.

The aim of this work was to study the geometries, electronic SW structures and its molecular complexes with nucleobases by DFTB methods. This study will shed more light on the nature of intercalations between a drug and DNA dominantly from the viewpoint of: charge transfer, dispersion and electrostatic forces. Hence, the study can help design new intercalators (drugs) to interact more with DNA.

2. COMPUTATIONAL METHODS

Calculations on isolated molecules and molecular complexes were performed with GAUSSIAN 98 package [45].

Both species were initially optimized with PM3 method and then the optimized structures were again optimized with density functional theory using the 6-31G* basis set. Full geometry optimizations and frequency calculations were performed and each species was found to be at minima, by having no negative values in the frequency calculation. The calculations gave internal energies at 0 K. In order to obtain gas phase free energies at 298.15 K, it is necessary to calculate the zero-point energies and thermal corrections together with entropies to convert the internal energies to Gibbs energies at 298.15 K [46,47] .

Frequency calculations on these structures verify that they were at true minima, and provided necessary thermal corrections to calculate H (Enthalpy) and G (Gibbs free energy). Finally, full optimizations and frequency calculations for each species were performed with the DFT/6-31G* [48,49].

The SW structure and geometry were optimized at the B3LYP level using the 6-31G* basis set. In order to find the most stable equilibrium structure for SW···Basepairs complexes, the initial guess structures are considered based on PM3 semi-empirical calculations followed by full geometry search based on Newton–Rapson procedure as implemented in GAMESS quantum chemistry code [50]. The

most stable geometries were achieved when the intercalator (SW) and base pairs (AT and GC) were situated in coplanar planes in such a way that the major system axes were parallel. There is special definition for the molecular geometries of DNA base pairs. In all cases, the QM-optimized geometries of the base pairs and intercalators were used for QM calculations. Thus, when the idealized geometries were utilized the interacting molecules were overlaid by their B3LYP/6-31G* optimized geometries, based on the least-squares fitting method. In the case of empirical potential calculations, either the subsystem geometries were relaxed by the empirical potential or the QM-optimized geometries were saved. This difference had an insignificant effect on the calculated energies.

The other one-electron properties (dipole moment, polarizability, energies of the frontier molecular orbital) were also determined at the B3LYP/6-31G* level. For charged species the dipole moment was derived with respect to their mass center, because for the non-neutral molecules the calculated dipole moment depends on the origin of the coordinate system.

The stabilization energies of selected complexes were determined by DFT calculations and calculated with a recently introduced method based on the combination of the approximate tight-binding DFTB with the empirical dispersion energy. The DFT methods are known to be inherently very deficient for stacking interactions as they basically ignore the dispersion attraction [51-53]. As a consequence their enlargement by an empirical dispersion term currently appears to be a very reasonable way to improve the major deficiency of the DFT method for the evaluation of the molecular complexes. It should also be mentioned that interaction energies were obtained as the difference between the complex energy and the combined energies of the molecules in isolation [54].

Processes in DNA environment depend on a delicate balance between stacking interactions, hydrogen bonding and hydration effects [55]. Hydration free energies could be calculated by implicit models like solvent reaction field [56] and Langevin dipole [57] methods, or by explicit models in conjunction with free-energy calculations and molecular dynamics simulations [58]. Due to complexity of these calculations, hydration effects will be evaluated in future studies.

3. RESULTS AND DISCUSSION

3.1. SW characteristics

The optimized structure, the atom numbering and the atom charges of SW before and after complex formation are shown in Figure1a and Figure1b, respectively. The equilibrium geometries of the SW subsystem were determined and confirmed by subsequent calculations of the vibrational frequencies. The geometrical optimizations were performed using the DFTB method and the significant computed geometrical parameters are available in Table 1. This table contains some significant geometrical values including: bond lengths, bond angles and dihedral angles for SW, before and after the complex formation (SW···AT and SW ···GC).

The atomic charge distribution in the SW is delocalized. The hydrogens 25 and 26 exhibited the highest positive charges which were the cause of their bonding to the nitrogen atom with high electronegativity. The most negative charges are Oxygens, because their contacted to hydrogen and

carbon is electropositive atoms. The presence of electronegative elements in SW facilitated its interaction with the DNA molecule through charge transfer. Actually, there are 2 kinds of interactions between CTTC and DNA; electrostatic interactions and dispersion interactions, being discussed in the next paragraphs.

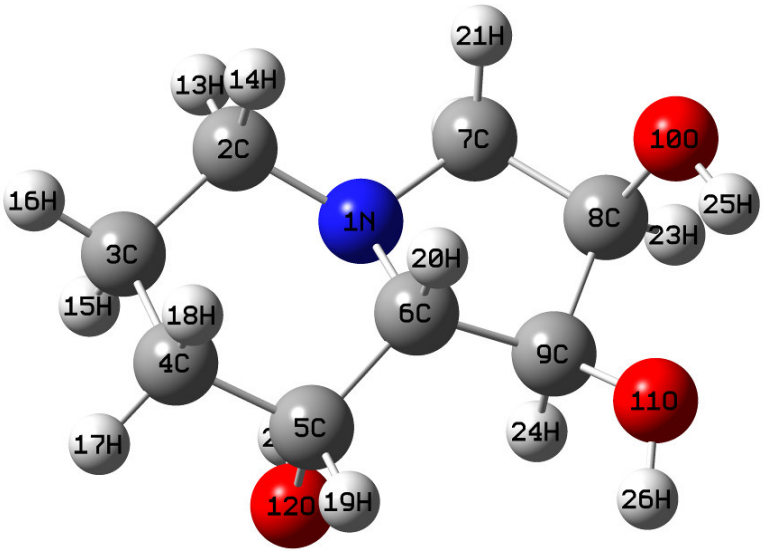


Figure 1a. The optimized structure and the atom charges of SW

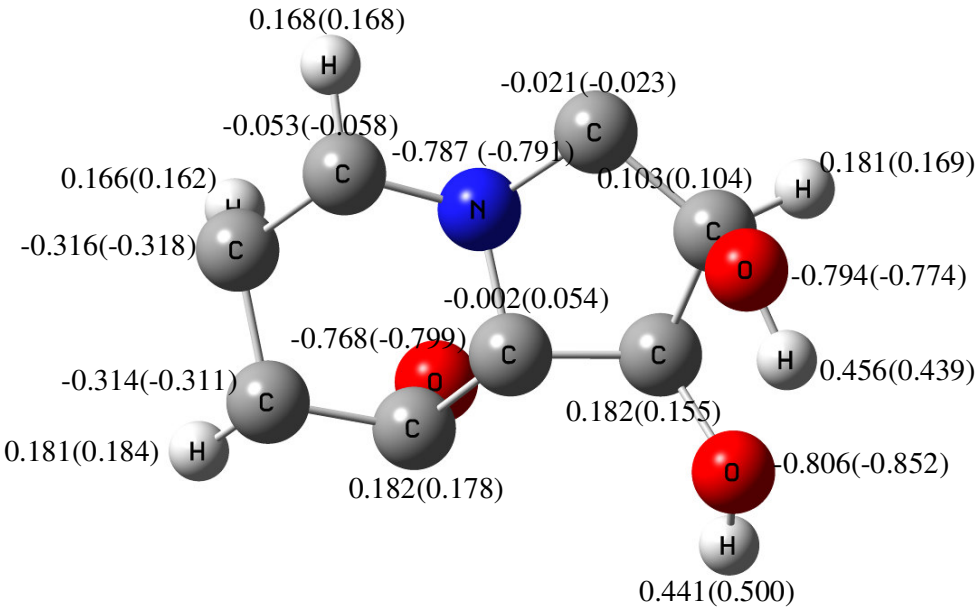


Figure 1b. The optimized structure and the atom charges of SW after the complex formation with GC and AT (Parentheses include the changes after the complex formation with AT)

Table 1. Significant computed geometrical parameters for SW before and after complex formation

Bond lengths	SW	SW-GC	SW-AT	Bond Angles	SW	SW-GC	SW-AT	Bond Dihedrals	SW	SW-GC	SW-AT
R(1,6)	1.4968	1.4654	1.4627	A(4,5,12)	112.7083	110.9181	110.4206	D(1,7,8,9)	-2.35	11.278	11.1624
R(1,7)	1.4871	1.4699	1.4715	A(6,5,12)	114.1475	110.7096	110.0161	D(1,7,8,10)	-125.19	-104.83	-104.975
R(5,6)	1.5414	1.5239	1.522	A(12,5,19)	101.4168	105.2413	105.2977	D(7,8,9,6)	-20.234	-32.567	-31.7459
R(5,12)	1.4046	1.4337	1.4402	A(9,8,10)	115.0617	109.1083	108.9884	D(7,8,9,11)	-142.20	-154.51	-152.113
R(5,19)	1.1148	1.0809	1.0798	A(11,9,24)	108.2411	110.3592	110.9493	D(10,8,9,6)	97.1476	82.8375	83.7864
R(8,9)	1.567	1.5343	1.5363	A(9,11,26)	105.9445	115.5607	115.1334	D(10,8,9,11)	-24.819	-39.106	-36.5803
R(8,23)	1.1149	1.081	1.082	A(5,12,27)	107.4502	110.9789	110.9494	D(23,8,9,6)	-140.26	-155.71	-154.852
R(9,24)	1.117	1.0806	1.0814	A(9,8,23)	110.0975	112.252	112.2579	D(23,8,9,11)	97.7721	82.3422	84.7811
R(8,10)	1.4087	1.4318	1.4299	A(8,10,25)	107.4259	110.2865		D(7,8,10,25)	169.6131	155.3163	150.1656
R(11,26)	0.9483	0.9512	0.9586	A(1,7,22)	107.5051	110.1416		D(9,8,10,25)	53.0125	42.237	36.7862
				A(8,9,11)	110.0553	107.5063		D(23,8,10,25)	-70.5799	-80.9225	-86.2991
								D(6,9,11,26)	54.1543		104.2021
								D(24,9,11,26)	-69.7993		-20.2818
								D(23,8,9,24)	-21.27		-37.5089
								D(6,5,12,27)	-58.5272		-44.7411
								D(17,4,5,12)	48.0459		55.9988
								D(4,5,12,27)	65.2116		75.9428

Table 2 depicts the one-electron properties (dipole moment and polarizability) and the energies of the frontier molecular orbital (HOMO and LUMO) of SW using the DFTB computational method.

The dipole moment which is the first derivative of the energy with respect to an applied electric field as a measure of asymmetry in the molecular charge distribution. The high values of the dipole moment and the polarizability present that the electrostatic and the dispersion contribution will play a key role in the interaction with the nucleobases.

Table 2. Dipole moment [D], polarizibility [B^3], HOMO and LUMO energies (in eV) of the drug, the bases and the base pairs

Compound	HOMO	LUMO	Dipole moment	Polarizability
AT	-8.64	3.01	1.28	213.2
GC	-7.35	2.74	2.51	223.4
SW	-5.88	1.17	0.94	84.8
A	-8.83	3.12	2.49	101.2
T	-9.53	2.94	3.88	89.1
G	-8.45	3.52	2.76	109.2
C	-9.93	3.01	6.12	80.4

3.2. Base pairs characteristics

The optimized structures of the adenine...thymine (AT) and guanine...cytosine (GC) based pairs in the Watson-Crick structures are visualized in Figures 2 and 3, respectively. Tables 3 and 4 show the significant computed geometrical parameters, using the DFTB method before and after the complex formation. In addition, Table 2 presents the one-electron properties (dipole moment and polarizability)

and the energies of the frontier molecular orbital (HOMO and LUMO) of the bases and the base pairs. From Table 2, it is clear that all the bases and base pairs are very poor electron acceptors (all LUMO energies are positive in contrast to the LUMO energy of SW which is negative).

The bases and the base pairs are apparently good electron donors and among the isolated bases the best one is guanine. This is in accordance with experimental and theoretical studies showing, that ultimate carcinogens primarily react with DNA at the N7 atom of guanine [59,60]. The electron donor ability of all bases is further magnified by base pairing. For example, the HOMO energy of guanine (-8.45 eV) increases by 1.1 eV upon pairing by cytosine.

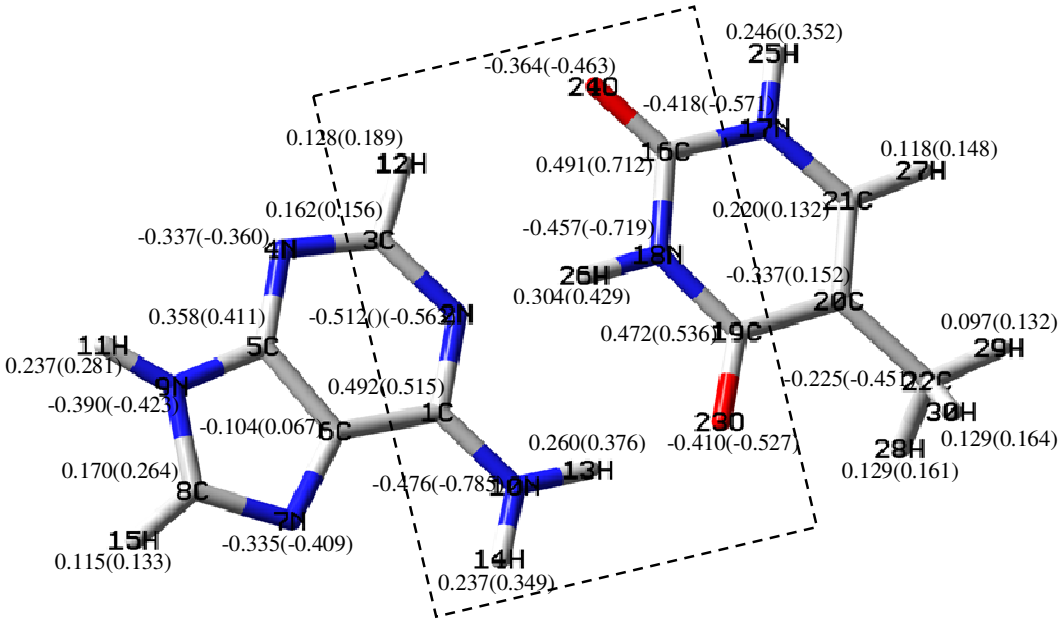


Figure 2. Optimized structure and charge of AT base pair & SW···AT before and after the complex formation (Parentheses include the changes after the complex formation)

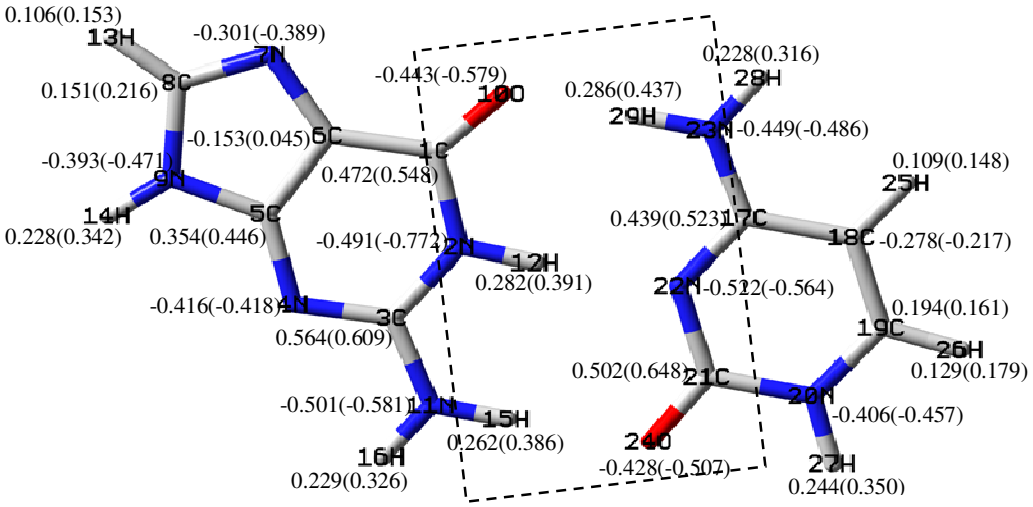


Figure 3. Optimized structure and charge of GC base pair & SW···GC, before and after the complex formation (Parentheses include the changes after the complex formation)

Furthermore, the high polarizability and dipole moment values of AT and GC (but more than those of SW) reveal that the electrostatic and dispersion contribution influence considerably the interaction with the intercalator.

According to Table 2 the LUMO energies of SW is very near the HOMO energies of AT and GC that clearly provide charge transfer interactions between SW and DNA.

Table 3. Significant computed geometrical parameters for AT and SW before and after the complex formation

Bond lengths	AT	AT-SW	Bond Angles	AT	AT-SW	Bond Dihedrals	AT	AT-SW
R(1,10)	1.3408	1.3276	A(2,1,10)	119.7	119.20	D(10,1,2,3)	180.0	179.9816
R(2,3)	1.3457	1.3437	A(1,2,3)	119.7	120.8289	D(10,1,2,26)	-0.0239	0.0339
R(2,26)	1.8226	1.8368	A(1,2,26)	123.2	123.5454	D(2,1,10,13)	0.0366	0.2759
R(3,4)	1.3293	1.321	A(3,2,26)	117.1	115.6258	D(2,1,10,14)	180.0	-179.482
R(3,12)	1.086	1.0687	A(2,3,12)	114.8	115.9057	D(1,2,3,12)	180.0	-179.961
R(10,13)	1.0199	0.9963	A(1,10,13)	120.7	119.2685	D(26,2,3,12)	0.0179	-0.0093
R(10,14)	1.006	0.9984	A(1,10,14)	118.6	123.2662	D(1,2,18,16)	-179.96	179.7012
R(16,18)	1.3799	1.3693	A(13,10,14)	120.6	117.4649	D(1,2,18,19)	-0.0098	-0.2035
R(16,24)	1.2142	1.2246	A(18,16,24)	124.4	123.3852	D(3,2,18,16)	-0.009	-0.2147
R(18,19)	1.3888	1.3666	A(16,18,19)	127.1	126.0917	D(3,2,18,19)	179.947	179.8807
R(18,26)	1.0455	1.0269	A(16,18,26)	115.9	115.9291	D(24,16,18,19)	-179.99	-179.949
R(19,23)	1.2293	1.2412	A(19,18,26)	117.0	117.9792	D(24,16,18,26)	-0.001	0.1028
			A(18,19,23)	120.8	119.9235	D(26,18,19,23)	0.0139	-0.2142

Table 4. Significant computed geometrical parameters for GC and SW before and after the complex formation

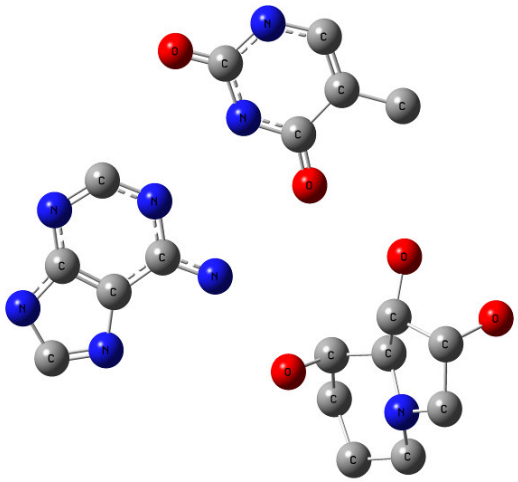
Bond lengths	GC	GC-SW	Bond Angles	GC	GC-SW	Bond Dihedrals	GC	GC-SW
R(1,2)	1.410	1.3954	A(2,1,10)	119.9	119.28	D(10,1,2,3)	-179.9	179.35
R(1,10)	1.2338	1.2382	A(1,2,3)	125.9	125.36	D(10,1,2,12)	-0.005	0.0704
R(2,3)	1.373	1.3641	A(1,2,12)	115.2	115.188	D(2,1,10,29)	0.0	-2.369
R(2,12)	1.032	1.0126	A(3,2,12)	118.9	119.4397	D(1,2,3,11)	-180.0	-178.5
R(3,11)	1.349	1.3449	A(2,3,11)	116.8	117.2218	D(1,2,12,22)	-0.5	-23.21
R(10,29)	1.765	1.8413	A(1,10,29)	127.2	130.4	D(1,2,17,22)	0.05	175.63
R(11,15)	1.020	1.0046	A(3,11,15)	123.1	122.148	D(12,2,3,11)	0.0203	0.665
R(11,16)	1.005	0.9914	A(3,11,16)	116.7	116.6878	D(1,10,29,23)	1.8	14.649
R(12,22)	1.910	1.9534	A(2,12,22)	177.1	174.94	D(2,3,11,15)	-0.084	-8.464
R(15,24)	1.915	1.840	A(11,15,24)	178.2	175.08	D(2,3,11,16)	-180.0	-173.6
R(17,22)	1.336	1.3314	A(10,29,23)	179.1	175.30	D(3,11,15,24)	-0.1	31.488
R(17,23)	1.335	1.3233	A(15,11,16)	120.3	119.4901	D(23,17,22,21)	-179.9	179.24
R(21,22)	1.357	1.352	A(22,17,23)	117.9	118.3368	D(22,17,23,29)	-0.019	-1.151
R(21,24)	1.229	1.2424	A(22,21,24)	124.6	123.5631	D(24,21,22,17)	-179.9	-179.7
R(23,29)	1.035	1.0096	A(17,22,21)	121.4	121.723			
			A(17,23,29)	120.6	120.3035			

SW cannot build up hydrogen bonds with DNA bases because of the lack of an appropriate side chain with oxygen or nitrogen atoms. As a consequence, for this drug, another stabilization factor has been proposed to build up an intercalation complex. This factor consists of the formation of charge-transfer complexes between the drug and the electron-rich DNA bases [2].

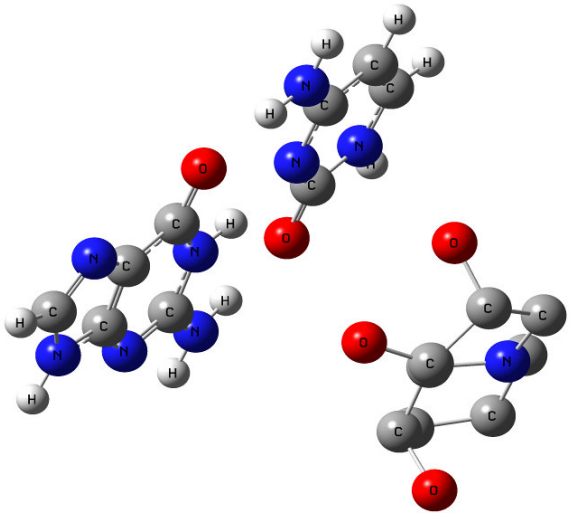
From the previous papers we can understand that the DFT method is more accurate. Moreover, the results concluded from the comparison of the DFTB method and the HF method indicates that these methods show close results and support each other.

3.3. Complex characteristics

The SW···AT and SW···GC optimized geometries are summarized in Figures 4a and 4b, respectively.



(a)



(b)

Figure 4(a,b). Optimized structures of SW···AT and SW···GC, respectively

The atom charge differences of SW, AT and GC are accessible in Figures 1 (a and b), 2 and 3. From Figure 1a and 1b, it is seen that the charge differences are not localized and are low in GC···SW and AT···SW, respectively which shows that the whole drug molecule participates for interacting with DNA base pairs. Although, in GC···SW charge differences are greater than AT···SW, special in dash mark area. Accordance to the high charge differences in the complexes conclude that in interaction between GC and SW is weak hydrogen bonding type (as were discussed in section 3.2), but in AT and SW charge differences is very law and hydrogen bonding don't appear [61].

Since the SW heteroatoms interact with the GC hydrogen in the zone, the charge changes are not important for the other heteroatom of the GC or AT bases pairs.

In general, a way for information collection regarding the electrons distribution is by computing the polarizability. This property depends on the second derivative of the energy relating to an electric field. Table 2 delineates the high SW, GC and AT polarizability values, supporting the fact that the dispersion energy is always important. Another way is dipole moment of the base pairs and the studied intercalator which is presented in Table 2. The significant polarizability and dipole moment values proved the existence of the dispersion and electrostatic interactions between DNA and SW. The polarizability and the dipole moment of the intercalator have the same effects on the interaction with DNA. Hence, a drug should be designed with high polarizability and dipole moment to increase the interactions between DNA and the drugs.

Furthermore the intercalation reaction between the SW and different double base pairs of DNA (A–T/A–T, A–T/T–A, A–T/G–C, A–T/C–G, C– G/G–C, C–G/C–G) was also studied by the PM3 method. Fig 5 is a sample related to this study. The double base pairs of DNA were built by the nucleic acid database of Hyperchem and their 3D geometry was optimized with PM3 method [62,63].

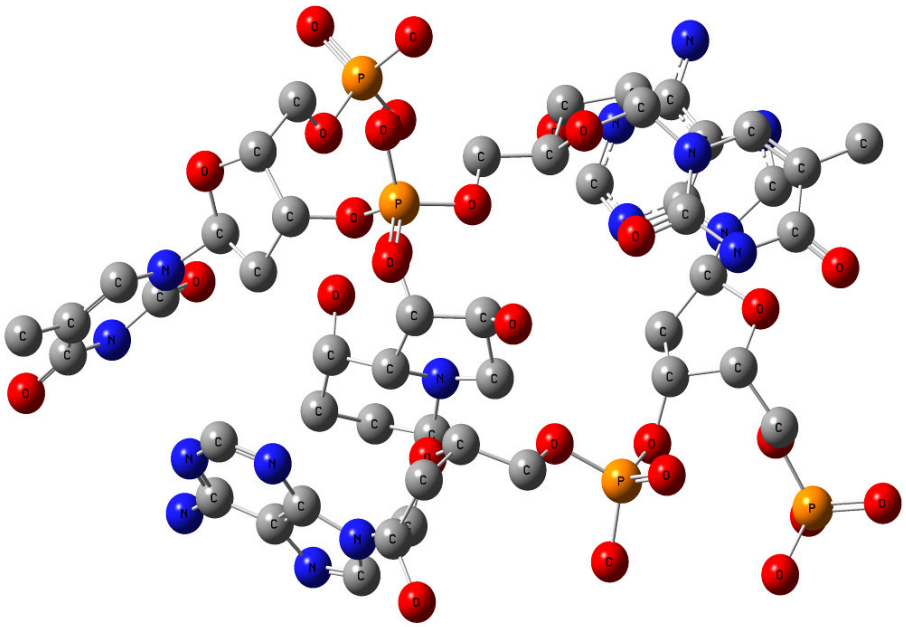


Figure 5. Optimized structures of SW with DNA double base pairs

4. CONCLUSIONS

1. SW is a good electron acceptor with high polarizability. In contrast, AT and GC base pairs are good electron donors. These outcomes are very favorable for aromatic stacking interactions between these two systems.
2. In designing a drug changes in the structure and addition of specific groups should be in order to increase values of the main parameters such as polarizability, dipole moment and interaction energy. With high values of these factors it can be concluded that the drug design is suitable.
3. It is evident that only the theoretical procedures properly cover the dispersion and polarization effects, and therefore these procedures were used for the study of intercalation processes and designing a drug that interacts more with DNA molecules.

ACKNOWLEDGEMENTS
We gratefully acknowledge the support of this work by the Institute of Petroleum Engineering, Tehran University Research Councils.

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