In this paper we have focused on the dielectric constant effect between various solvents with theoretical model in the biochemical process. Thereby, AAA, UUU, AAG and UUC triplex sequences have been optimized in water, methanol, ethanol and DMSO with proposed SCRF Model of theory. The solvation of biomolecules is important in molecular biology since numerous processes involve to interacting a protein with changing of solvent-molecule. The hydrogen bond is one of the important predictions of structural and functional in biochemical and biophysical of biological complexes such as proteins. mRNA-tRNA pairing as a fundamental step in protein
synthesis is a complex process controlled by hydrogen bonding between two anti-parallel trinucleotides, namely the mRNA codon and the tRNA anticodon.

In order to determine the optimized structural biology including of bond lengths, bond angles and dihedral angles energies, dipole moments and other properties of codons and anticodon, we have performed ab initio calculations of Quantum Mechanics (QM) at HF/sto-3G, 3-21G, 6-31G levels in gas phase and a few solvents with different dielectric constants via the SCF method using the GAUSSIAN 98 software package. Optimization at the HF/6-31G level has yielded results in better agreement with the experimental data.

INTRODUCTION

The Watson-Crick type base pair formation is fundamental for molecular recognition in the duplex formation of nucleic acids [1, 2]. The processes of transcription from DNA to mRNA [3], and of translation from mRNA to protein via tRNA [4] are also based on the formation of the Watson—Crick type base pairs.

Each amino acid in a protein is specified by a group of the three adjacent nucleotide bases, denoted a codon, on the messenger RNA (mRNA) strand. Three special nucleotide bases in the tRNA molecule, the anticodon, interact with the three complementary codon bases in the mRNA molecule through hydrogen bonds and joining of the amino acid into a chain is realized inside the ribosome. In a process called translation, the mRNA molecule directs the collection of amino acids into the specific linear sequence characteristic of a given protein [5].

Theoretical nucleic acid conformational investigations have, thus far, mainly been concerned with the elucidation of the factors that govern sequence-dependent conformational properties.

Codon-anticodon pairing is not merely a simple process controlled by hydrogen bonding between two anti-parallel trinucleotides, namely the mRNA codon and the tRNA anticodon. For example, peculiarities of the codon-anticodon interaction such as the absence of non-canonical base pairing at the first two positions of the codon cannot be explained just by the internal stability of the codon-anticodon mini helix and the influence of the tRNA anticodon loop. It is known that a wide variety of non-canonical base pairs is observed in different regions of the double helices of RNA molecules [6-9], and even in different positions of the anti-codon-anticodon mini helices [8,10]. There is also a series of indications that the translation of the codon can depend on adjacent codons (codon context effects [11-13]).

Although we know which anticodon-codon complexes are recognized as “correct,” we have never understood why only they are acceptable. Crick (1966), based on the emerging structure of the genetic code and base pair stereochemistry, and proposed his famous wobble rules for identifying correct duplexes. He proposed that only canonical base pairing should occur at the first and second codon positions, and that certain wobble pairing would be possible at the third codon position. In succeeding years these general rules have been amply confirmed, although the range of acceptable wobble pairs has been expanded (Osawa et al., 1992; Boren et al., 1993; Inagaki et al., 1995). There has also been progress towards an understanding of how nucleoside modifications affect wobbling (e.g., Agris, 1991; Björk, 1992, 1998; Osawa et al., 1992; Yokoyama & Nishimura, 1995; Curran, 1998).

In fact, some of these mispaired complexes are just as stable as duplexes that contain only correct base pairs. Clearly, both correct and wrong codon-anticodon duplexes can be stable in solution. Notice that ribosomal proofreading, which can in principle amplify small energetic differences (Hopfield, 1974; Ninio, 1975; Kurland et al, 1990; Yarus, 1992), cannot distinguish duplexes that have essentially the same stabilities. Therefore, in addition to using a proofreading mechanism, ribosomes must rely on features other than duplex stability as predicted from solution and structural studies.
In the solution and while interacting with other materials, nucleic acids have also shown to adopt conformations not at all similar to the original Watson and Crick model (Srinivasan and Olson, 1987; Jaworski et al., 1987; Wu et al., 2002). Rigid body docking and static models have been used to examine the codon–anticodon–ribosome interactions, and ternary complex initial selection. Smaller scale molecular dynamics simulation studies of cognate codon–anticodon interactions in the absence of the ribosome have also been performed. (Sanbonmatsu and Joseph, 2003)

And mean free energy generated from the secondary structure of RNA sequences of varying length and composition has been studied to show that some nucleotide sequences found in biologically active organisms do relate to the free energy of their structures. Recently, a theoretical model based on similarity for studying RNA base pairings has been built up to analysis both Watson–Crick and non-Waston–Crick pairings. And some theoretical considerations concerning the capability of the genetic code to repair dangerous mutations contribute to the ongoing debate (Patrizia et al.,1996). The impact of base-pair interactions to the RNA folding and biological functions is quite prevalent. Codon–anticodon interactions are involved in the discrimination between the correct and incorrect aminoacyl-tRNAs. Hydrogen bonding, steric fit, and base-pair stability may be the main aspects that influence the whole process [14].

Water is the natural medium of all biological reactions, participating in different processes involving the living cell. Particularly, several structural features that are necessary for the biological functions of nucleic acids, such as DNA double helix formation or RNA folding and nucleic acids base pairing, are dependent on their interactions with surrounding water .The hydration of nucleic acids is controlled by the interaction of water molecules with various hydrophilic sites such as phosphates, bases and sugars.

Water is a highly polar molecule which can be simultaneously an acceptor and a donor of H-bond via the interactions occurring through its oxygen or hydrogen atoms, respectively, with the nucleic acid constituents.

Computational methods allow for the visualization of large amounts of structural data and the generation of related conformations for statistical and dynamic analyses. The application of these methods to systems of biological interest has advanced tremendously in recent years to encompass models that describe local conformational effects with great precision: such as quantum mechanical (QM) studies of the effect of substituent modifications, methods that perform statistical energy-guided conformational searches such as energy minimization, Monte Carlo (MC) and molecular dynamics (MD) simulations, and algorithms that aim to describe the collective structural constraints that influence macromolecular tertiary structure, folding pathways and the energetics of supercoiling.

Theoretical backgrounds
The most common type of ab-initio calculation is called Hartree-Fock calculation (abbreviated HF), in which the primary approximation is called the mean field approximation. This means that the coulombic electron-electron repulsion is not explicitly taken into account, however, its average effect is included in the calculation [15].

In the density functional theory (DFT), electron correlation is introduced through the Kohn and Sham method [16, 17], based on the combinations of some density functional (exchange, correlation). In the present work, the hybrid functional Beck’s three parameters (B3) [18] combined with the gradient corrected correlation functional of Lee-Yang-Parr [19] also denoted B3LYP is used.

Computational methods
The studies of Hydrations of nucleobases were a subject of numerous theoretical studies using Monte-Carlo, molecular dynamics, and quantum-chemical approaches within the...
continuum model. Such information may by obtain only within the super molecules approach using high level ab initio methods. Also so far, no theoretical study has been done on pairing behaviors of these bases. Thus by this study we intend to propose the first detailed mechanism and investigate the effects of solvent surrounding them on changing of succession of amino acids.

A quantum mechanical (QM) calculation was performed to verify the nature of the minimum state of the stationary points reached after geometry optimization. The geometries of the AAA, UUU, AAG and UUC have been optimized by ab initio and DFT calculations using the standard STO-3G, 3-21 G, 6-31G and 6-31G* basis sets, in Hartree-Fock (HF) and B3LYP levels. The calculations have been performed by using the Gaussian 03 suite of program.

RESULTS AND DISCUSSION

Nucleic acid bases contain a row of N and N-H groups, which provide a range of possible hydrogen-bonded with water molecules. In all of these the water molecule is bonded to AAA, UUU, AAG and UUC triplex sequences hydrogen bond (OH...N or NH...O). Firstly, the complexes were fully optimized with HF and DFT (BLYP and B3LYP) methods at 3-21G, 6-31G and 6-31G* basis sets and we have located the minima on the nucleobases potential energy surface.

Optimization parameters such as: dipole moments and energies yields molecular geometries in good agreement with experimental values and those previously obtained theoretically.

The results in Table 1 show that, with increase of dielectric constant from vacuum to cyclohexane, ethanol, methanol, DMSO and water, the dipole moment of each model increases by different quantum mechanic levels.

A dipole in the molecule will induce a dipole in the medium, and the electric filed applied by the solvent dipole will in turn interact with the molecular dipole, leading to net stabilization. These parameters represent the subtle structural changes of the triplets are not statistically correlated because the distributions of subtle structural changes of different triplets are very different, and the contributions of dedicated structure changes should be analysed individually (Fig.2). The values of calculations in table 1 show that the interactions between water molecules and triplets reduce the energy of the integer system. The only exception is non-bond dispersion energy; it may imply that in aquatic solution, import of polarized water molecules reduces the polarization rates of triplets. The significance levels of parameters reveal the changes of solvent groups are significant.

The effect of solvent on stabilization of triplex bases indicates interesting results and play major roles in their activities. The standard approach of the PCM (by SCRF method) for nucleobases with different basis sets, as is used here appears to be a good first step in the theoretical investigation on the effect of solvent. In this paper, we have presented the solvation of the complexes. The influence of dielectric constant on the standard geometry optimization of AAA, UUU, AAG and UUC triplex sequences in H2O, C2H5OH, CH3OH and DMSO solvents have investigated. We have shown that relative energies (ΔE) of triplex bases in solution are smaller than gas phase, which is due to interactions in solution is larger than gas phase and it seems for all different sequences that the influence of aquatic solution to mRNA-tRNA triplets is almost the same (Table 1).

The interaction energies of the complexes with increasing dielectric constant of solvent decrease at HF, BLYP and B3LYP methods. The charts of AAA and UUU triplex bases almost are linear but we have not seen this form for AAG and UUC triplex sequences. Also, the non-linear chart in the antisenses sequences (AAG and UUC) at heavy basis set of 6-31 G* turnout linear (Fig.3). The results obtained from density functional theory are larger than those obtained from Hartree–Fock calculations because correlation energies are considered in DFT method. However, the accuracy of BLYP and B3LYP calculations has been considered as insufficient for base triplets interactions.
Because the increase of dielectric constant in water molecules that are arranged around the hydrophilic part of chain of amino acid, we have found the optimized parameters better than other solvents.

Also, from these calculations we result that the effect of dielectric constant of solvents is important to displacing of amino acids sequences on codon-anticodon residues pairing in proteins and it will be causes some mutations in human body.

Conclusion

1. For the compound studied, the most important intermolecular interaction between nucleobases and solvent molecules employ different geometrical models in the crystalline structures. These interactions have been approximated by explicitly adding the nearest neighbors into the calculations. Interaction with solvent molecules has caused deformation of the intermolecular geometry of the nucleobases which can be described by assuming the resonance form into the total structure of the bases.

2. The comparison between optimized structures investigates stability of chain amino acids in theoretical levels. We have performed HF and DFT quantum mechanic methods of good quality on the AAA, UUU, AAG and UUC triplex sequences in Water, Ethanol, Methanol, and DMSO solvents with different basis sets.

Based on the obtained results and stabilized structures, we conclude that it may be dielectric constant effect of solvents have been caused to displacing of amino acids sequences on codon-anticodon residues pairing in proteins and it will be indicate some changes in biological ambient.

3. Based on the analysis of the physico-chemical properties of mRNA and tRNA, Jean Lehmann (2000) pointed out that nature of the codon–anticodon interaction can explain the volume of the corresponding amino acids. Peptide bond formation may exist between two successive amino acids during translation. And the nature of codon–anticodon may be sufficient to explain the origin of comparison the energies of mRNA and tRNA triplets in vacuum, and those in aquatic solution show significant differences.

4. Presence of active centers in base triplex may be important in the recognition code mechanism involving tRNA. We are now working towards an ab initio confirmation. The calculated group-group bond indices and molecular valences agree with these features. The change of nucleotide in codon-anticodon shows complexity which may lead to different biological functions. As a matter of fact, the energies can provide some valuable information for binding stabilities of pairing in proteins and it will be causes some mutations in human body.
Fig. 1. geometry optimization of (a)AAA, (b)UUU, (c) AAG and (d)UUC triplex sequences by showing of active centers.
Table 1. Values of dipole moment and relative energy in AAA, UUU, UUC and AAG triplex sequences in HF and DFT (BLYP and B3LYP) methods at various ambient.

<table>
<thead>
<tr>
<th>Solvent (dilute)</th>
<th>PARAMETER</th>
<th>HF</th>
<th>BLYP</th>
<th>B3LYP</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3-21g</td>
<td>6-31g</td>
<td>6-31g*</td>
<td>3-21g</td>
</tr>
<tr>
<td>AAA dipole</td>
<td>40.9237</td>
<td>40.4713</td>
<td>59.2331</td>
<td>-------</td>
</tr>
<tr>
<td>UUC dipole</td>
<td>65.1489</td>
<td>66.0421</td>
<td>64.8689</td>
<td>24.53</td>
</tr>
<tr>
<td>Cyclohexane (2.02)</td>
<td>69.5254</td>
<td>78.9865</td>
<td>78.0468</td>
<td>63.3546</td>
</tr>
<tr>
<td>UUC dipole</td>
<td>35.2009</td>
<td>37.8514</td>
<td>33.1146</td>
<td>23.6523</td>
</tr>
<tr>
<td>Ethanol (2.55)</td>
<td>73.3946</td>
<td>80.2768</td>
<td>78.4816</td>
<td>-------</td>
</tr>
<tr>
<td>UUC dipole</td>
<td>35.3862</td>
<td>37.7185</td>
<td>33.2293</td>
<td>23.7455</td>
</tr>
<tr>
<td>Methanol (2.25)</td>
<td>77.9591</td>
<td>79.7979</td>
<td>78.8884</td>
<td>-------</td>
</tr>
<tr>
<td>UCC dipole</td>
<td>35.1363</td>
<td>37.1399</td>
<td>33.2979</td>
<td>23.8232</td>
</tr>
<tr>
<td>DMSO (4.37)</td>
<td>31.8664</td>
<td>83.1767</td>
<td>79.2766</td>
<td>-------</td>
</tr>
</tbody>
</table>
Fig. 2. Comparison of the dipole moment (debye) (a) AAA, (b) UUU, (c) AAG and (d) UUC triplex sequences versus dielectric constant obtained from HF and DFT (BLYP and B3LYP) methods at different basis sets.
Fig. 3. Variation of relative energy (kcal/mol) (a)AAA, (b)UUU, (c) AAG and (d)UUC triplex sequences versus dielectric constant obtained from HF and DFT (BLYP and B3LYP) methods at different basis sets.

REFERENCES