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Review

Theoretical study of inclusion complexation of 3-amino-5-nitrobenzisothiazole with β-cyclodextrin

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ABSTRACT

The inclusion process involving β-cyclodextrin (β-CD) and 3-amino-5-nitrobenzisothiazole (ANBT) has been investigated by using the MM+ force field, AM1, PM3, HF and B3LYP theories. In this study we took into account only the stochiometry1:1. The complexation and interaction energies for both orientations considered in this research are reported. All quantum computational methods gave the A orientation as the most favorable in which the guest molecule is totally embedded in the hydrophobic cavity of the cyclodextrin with the NO2 group located near the primary hydroxyls of the β-CD and the NH2 group near the secondary hydroxyls with no hydrogen bonding formation. The negative complexation and interaction energies calculated suggest that the inclusion complexes are stable. HOMO and LUMO orbital investigations confirm the better stability of the A orientation.

Contents

1. Introduction

Inclusion complexation is the focus of current host–guest chemistry and supramolecular chemistry [1,2]. Cyclodextrins (CDs), the most prominent host molecules up to now, cyclic oligosaccharides are composed of glucopyranose units and can be characterized as a truncated cone structure with hydrophobic interior and hydrophilic exterior [3] (see Fig. 1). These amphiphilic molecular structures of CDs are easy to form inclusion complexes with many of organic, inorganic and biological compounds without covalent bond. The resultant inclusion complexes can induce modification of the physicochemical properties of guest molecules (such as water solubility and solution stability) [4–6]. Therefore pharmaceutical application of CDs as additives and drug-complexing agents had attracted growing attention in recent years [4–7]. In addition, CDs can mediate many organic reactions giving a good model of mimicking enzymes [6,7] and have molecular recognition property to identify the tiny difference of isomers [8,9]. Due to the limitation of the experimental methods, molecular modeling is very popular in CDs chemistry [10–19]. The derivatives of benzisothiazole are widely used in medical and biomedical fields [20–22]. If amino group is inside the cavity of β-CD, its behavior may be affected by the formation of complex with β-CD.

Recently, R. Rajamohan and al. [23] have studied the encapsulation of ANBT in β-CD and it was observed that the nitro-aryl group is present in hydrophobic cavity of β-CD, but no information about the orientation of ANBT in β-CD cavity was given.

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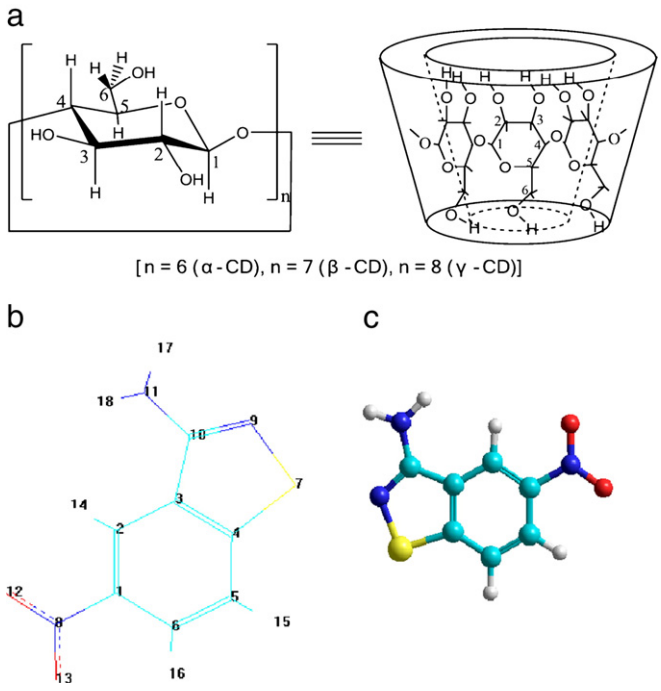

Fig. 1. Molecular structures of β-CD (a), ANBT (b) and B3LYP/6-31G* optimized structure of ANBT (c).

In this paper, several levels of calculations were carried out. In the first part, we use the MM+ force field of molecular mechanics in order to research the lowest energy structure of the inclusion complex. In the second part of work, superior levels of calculations were made such PM3, AM1, single point HF and DFT calculations in order to approach the ideal geometry and provide further insight into the different complexation properties of the guest molecule.

However, because of the limitation of our computer, it can hardly calculate the interactions of cyclodextrins systems in aqueous solution.

2. Computational methods

The inclusion model can be seen in Fig. 2. The glucosidic oxygen atoms of β-CD were placed onto XY plane; their centre was defined as the origin of the coordinate system. The guest molecule placed on the Z axis was allowed to approach the β-CD cavity from the wide rim at a distance of 8 Å which separates the β-CD equatorial plane and the labeled carbon atom C4 in ANBT (Fig. 2). The inclusion process emulation was then achieved along the Z axis to −8 Å with a step of 1 Å. The structure generated at each step was then optimized, allowing them to change from the initial conformations while keeping the movement of the reference atoms and β-CD structure totally restricted. In order to find an even more stable structure of the complex, each guest molecule is calculated for all of the structures obtained by scanning θ, clock wisely circling around Z-axis, at 30° intervals from 0° to 360°.

Complexation energy upon complexes between ANBT and the β-CD is calculated for the minimum energy structure according Eq. (1).

$$E_{complexation} = E_{complex} - \left(E_{free\ ANBT} + E_{free\ \beta-CD}\right) \quad (1)$$

where $E_{complex}$, $E_{\beta\text{-CD}}$ and E_{ANBT} represent respectively the total energy of the complex, the free optimized β-CD and the free optimized ANBT energy. The magnitude of the energy change would be a sign of the driving force toward complexes.

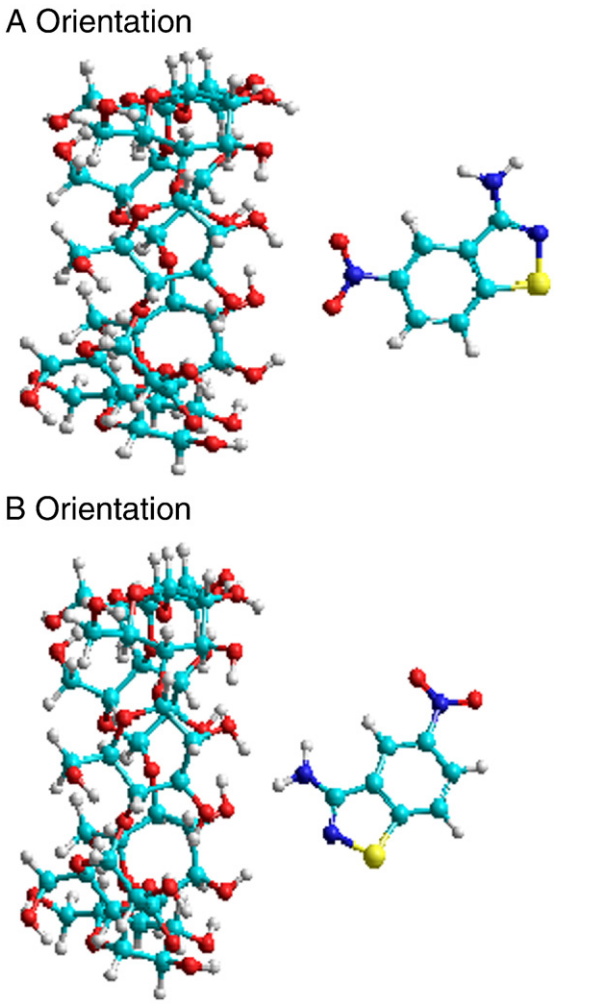

Fig. 2. The proposed structures of ANBT/β-CD complex for A and B orientations.

The quantification of the interaction between ANBT and β-CD in these most stable geometries is represented by the energetic term E interaction which was calculated using Eq. (2).

$$E_{interaction} = E_{complex} - \left(E_{\beta-CD\ in\ complex} + E_{ANBT\ in\ complex}\right) \quad (2)$$

In this equation $E_{\beta\text{-CD in complex}}$ and $E_{ANBT\ in\ complex}$ correspond respectively to the single point energy of the β-CD and ANBT in the optimized complex.

The initial structure of β-CD is built with CS Chem3D Ultra (version 10, Cambridge software) from the crystal structure [24] and fully optimized by PM3 method without imposing any symmetrical, while the initial structure of ANBT was constructed by module builder of Hyperchem then optimized with B3LYP method at 6-31G* level.

The more stable complexes found by MM+ calculations were optimized by PM3 and AM1 methods without imposing any symmetrical restrictions. The density functional theory (B3LYP) and Hartree-Fock (HF), which considers the electron correlation and high precision of energy calculations [25,26], are applied to calculate the single point energies of the inclusion complexes. A small and medium basis sets corresponding respectively to 3-21G and 6-31G were chosen. All calculations were carried out using Hyperchem 7.51 [27] and Gaussian 03 W version 6.0 [28] packages respectively for molecular and quantum mechanics methods.

3. Results and discussion

3.1. Force field calculations

All the optimized structures obtained by scanning the θ angle, from 0 to 360° at 30° intervals, and the coordinate Z, from −8 to +8 Å at 1 Å intervals, were used to find the most favorable approach of the ANBT/β-CD. Two E minima are found at Z = −1 Å, θ = 140° and Z = −3 Å, θ = 300° for the A orientation (Group NO2 orientated to the centre of mass of β-CD) and the B orientation (Group NH2 Aromatic ring orientated to the centre of mass of β-CD). The models are shown in Fig. 3. We noticed that the curves reported for the variation of Van der Waals (VdW) energy contribution are pretty similar to those of complexation energy with practically the same magnitude of energy changes for all cases. Therefore, we may conclude that the driving forces of the complexation process were mainly VdW interactions between guest and host molecule.

The results summarized in Table 1 for the most stable structures obtained by MM+ study confirm that both complexation and interaction energies are in favor of the A orientation and the energy difference of the complexes in the two orientations correspond respectively to −1.71 and −2.8 Kcal /mol. Moreover, the similarity in the magnitude of the energetic contribution of VdW interaction and the complexation energy is an indication that the driving forces responsible of the stability of the inclusion ANBT/β-CD complexes are VdW interaction.

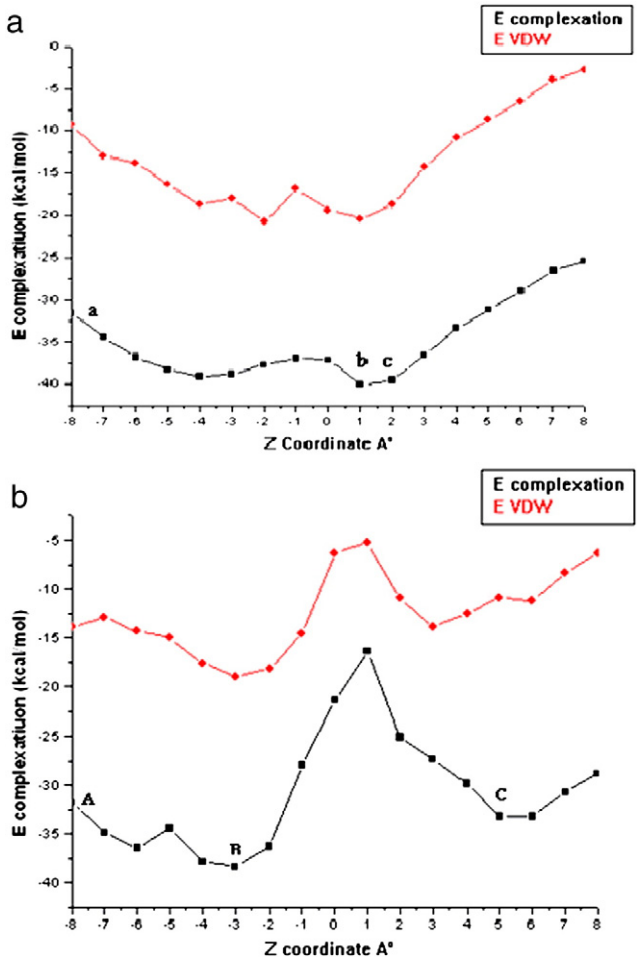

Fig. 3. Stability energies of the inclusion complexation of ANBT into β-CD at different positions (Z) and models: (a) A orientation, and (b) B orientation orientations. Point a, b, c represent Za = −8 Å, ZB = 1 Å, and ZC = 2 Å respectively. Point A, B, C, d represent Za = −8 Å, Zb = −3 Å, and Zc = 5 Å respectively.

Table 1
Complexation, interaction and VDW energies (kcal/mol) at the minimum energy for both orientations calculated by MM+ method.

Energetic terms	A Orientation	B Orientation	ΔE
E complexation	−40.09	−38.38	−1.71
E interaction	−41.85	−39.05	−2.80
E VDW	−20.74	−18.98	−1.76

All energetic values are in Kcal/mol.
ΔE is the relative energy difference of the optimized complexes in 'B' and 'A' orientation, ΔE = E complexation (A) − E complexation (B).

3.2. Semi empirical and quantum mechanical calculations

Unfortunately, molecular mechanics methods do not treat explicitly the electrons [29]; therefore they cannot predict electronic properties of molecules. Also, it may not accurately describe the geometries or energetic of intermolecular interactions if a force field for a molecule is not available or not very well defined. Hence, to

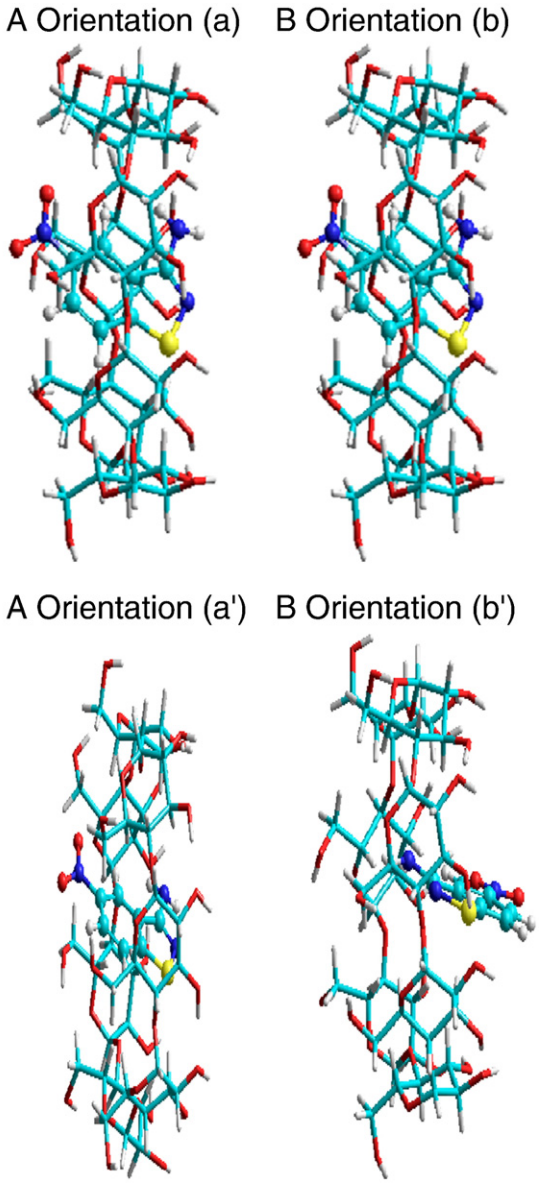

Fig. 4. Geometrical structures of the most stable ANBT/β-CD inclusion complexes. a) and b) correspond respectively to A and B orientation from PM3calculation. a') and b') correspond respectively to A and B orientation from DFT calculation.

verify the reliability of our approach and to be consistent with experiment we have used quantum mechanical methods.

The above equilibrium geometries of both ANBT/β-CD were re-optimized by semi empirical AM1 and PM3 methods, then DFT/B3LYP and ab initio HF single point calculations were performed [30,31]. The energy minimized structures obtained from PM3 and B3LYP calculations are illustrated in Fig. 4.

Semi-empirical calculations were performed starting from the structures of minimal complexation energy obtained in the previous MM+ study. The energy E of the complex obtained can reflect the stabilization structures after complexation according to Table 2. Complexation energy is in favor of the A orientation by −2.06 Kcal/mol and −4.95 Kcal/mol respectively for PM3 and AM1 methods. The same result is also obtained with the B3LYP and HF single point calculation in which the energy difference becomes respectively −3.61 and −4.91 Kcal/mol for 3-21G* basis set and −3.43 and −2.99 Kcal/mol for 6-31G* basis set.

The main feature of the favorable structure obtained by PM3 and AM1 shows that The ANBT in the A orientation entered full in β-CD hydrophobic cavity of β–CD .The NO2 group faces the primary hydroxyls of β-CD and the NH2 group faces the secondary hydroxyl. In the B orientation the ANBT is located adjacent to the cavity of β–CD. In the two A and B orientations there is no interaction between the NH2 and NO2 groups of ANBT and the–OH groups of β –CD (Fig. 4). This contestation is in good agreement with experimental results [23].

Besides, the geometrical changes of β-CD after guest inclusion are shown in Fig. 5. We found that dotted lines lengths in Fig. 5b are shorter than Fig. 5a. The round cavity of β-CD turns into an oval-shaped cavity .Atoms O-49 and O-65 are part of the hydroxyl groups of the top rim of β-CD. Atoms O-47 and O-68 are the part of the hydroxyl groups of bottom rim of β-CD. Therefore, the hydroxyl groups of the top/bottom rim of β-CD play a significant role in binding the ANTB.

Furthermore, the (E_{HOMO}–E_{LUMO}) gap is an important stability index [32] and chemicals with larger (E_{HOMO}–E_{LUMO}) values tend to have higher stability, so we investigated the electronic structure of the complexes in the two orientations using AM1 and PM3 methods.

The results are reported in Table 2. In fact, with the increase of the (E_{HOMO}–E_{LUMO}) gap for the complexes formed in the A orientation, we present a new confirmation that ANBT/β-CD inclusion complexes are more stable when NO2 group of ANBT enters the cavity by its wide side, which agrees well with the calculated results of the complexation energies discussed above.

Table 2
Energies and HOMO–LUMO calculations using AM1 and PM3 methods and single point energy evaluated at HF and B3LYP for ANBT/β-CD inclusion complexes.

Energetic terms	A Orientation	B Orientation	ΔE^d
PM3			
E^a complexation (Kcal/mol)	−59.77	−57.71	−2.06
E^a interaction (Kcal/mol)	−54.30	−52.13	−2.17
E^b_{HOMO} (eV)	−7.19	−7.12	
E^c_{LUMO} (eV)	−0.45	−0.54	
(E_{HOMO}–E_{LUMO}) gap (eV)	−6.74	−6.58	
AM1			
E^a complexation (Kcal/mol)	−115.20	−110.25	−4.95
E^a interaction (Kcal/mol)	−90.21	−88.95	−1.26
E^b_{HOMO} (eV)	−7.07	−7.01	
E^c_{LUMO} (eV)	−0.32	−0.50	
(E_{HOMO}–E_{LUMO}) gap (eV)	−6.75	−6.51	
HF/3-21G*			
E^a complexation (Kcal/mol)	−883.65	−880.04	−3.61
B3LYP/3-21G*			
E^a complexation (Kcal/mol)	−870.03	−865.12	−4.91
HF/6-31G*			
E^a complexation (Kcal/mol)	−879.29	−876.30	−2.99
B3LYP/6-31G*			
E^a complexation (Kcal/mol)	−866.39	−862.96	−3.43

E^a is the HF energy, E^b energy of the Highest Occupied Molecular Orbital, E^c energy of the Lowest Unoccupied Molecular Orbital.
ΔE^d is the relative energy difference of the optimized complexes in A and B orientation, ΔE^e = E complexation (A) − E complexation (B).

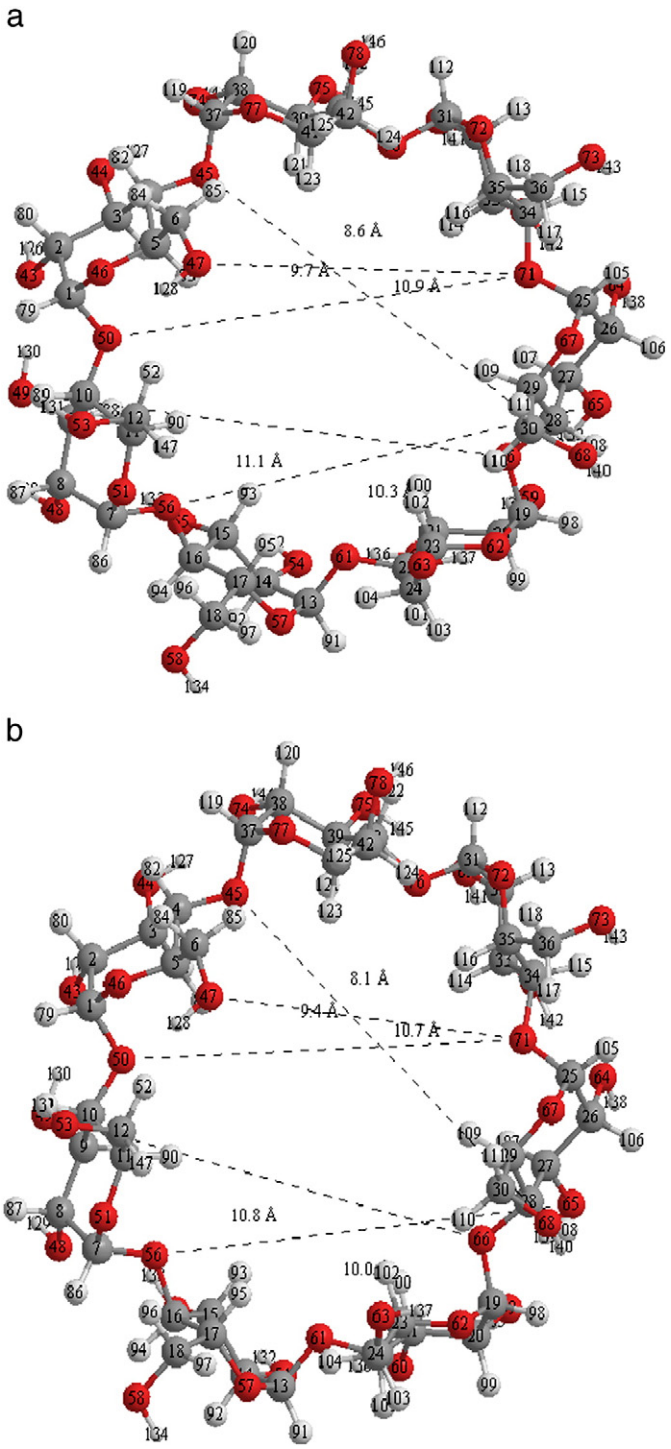

Fig. 5. PM3 optimized structure of β-CD (a) and structure of β-CD after guest inclusion (b). Fig (b) is the A orientation after removal of the structure of the ANTB. The solid lines length represents the distance between numbered atoms. The glycosidic oxygen atoms of β-CD number are O-45, O-56, O-66 and O-71. Gray balls represent the carbon atoms, red balls represent oxygen atoms.

3.2.1. Charge transfer

Liu and Guo suggest that charge transfer interactions play a relevant role in the stabilization of their inclusion complexes [33]. The

Table 3
Milliken charges (e) of the heavy atoms of ANBT, charge transfer of the two orientations calculated by AM1, PM3 and B3LYP/6-31G*methods.

Atoms	ANBT	A orientation	B orientation
	AM1/ PM3/B3LYP/6-31G*	AM1/ PM3/B3LYP/6-31G*	AM1/ PM3/B3LYP/6-31G*
C1	−0.10/−0.34/0.21	−0.11/−0.421/0.27	−0.12/−0.43/0.24
C2	0.23/0.26/0.36	0.17/0.20/0.13	0.18/0.20 /0. 25
C3	−0.19/−0.20/−0.60	−0.16/−0.14/ 0.15	−0.16/−0.15/−0.01
C4	−0.17/−0.11/−0.46	−0.17/−0.17/ −0.40	−0.17/−0.17/−0.51
C5	0.05/0.06/0.05	0.07/0.04/0.01	0.06/0.04/0.07
C6	0.12/0.13/0.26	0.11/0.14/0.09	0.11/0.14/0.19
S7	0.38/0.26/0.69	0.32/0.27/0.60	0.31/0.27/0.69
N8	0.37/0.98/−0.12	0.51/1.32/0.08	0.50/1.32/0. 15
N9	−0.33/−0.30/−0.75	−0.29/−0.26/−0.60	−0.27/−0.26/−0. 73
C10	0.16/0.00/0.67	0.14/−0.01/0.30	0.14/−0.01/0.60
N11	0.15/0.33/−0.17	0.09/0.23/−0.0.2	0.09/0.26/−0. 17
O12	−0.35/−0.55/−0.35	−0.34/−0.58/−0.32	−0.35/−0.62/−0.37
O13	−0.33/0.56/−0.33	−0.36/−0.61/−0.28	−0.33/−0.59/−0.40
H14	0.00/0.00/0.00	0.00/0.00/0.00	0.00/0.00/0.00
H15	0.00/0.00/0.00	0.00/0.00/0.00	0.00/0.00/0.00
H16	0.00/0.00/0.00	0.00/0.00/0.00	0.00/0.00/0.00
H17	0.00/0.00/0.00	0.00/0.00/0.00	0.00/0.00/0.00
H18	0.00/0.00/0.00	0.00/0.00/0.00	0.00/0.00/0.00
Charge transfer	−0.01/−0.01/−0.54	−0.02/0.01/0.01	−0.01/0.00/0.00

Milliken charges of the heavy atoms of ANBT, charge transfer of the models are summarized in Table 3 by AM1, PM3 and B3LYP/6-31G* methods. The data show that the β-CD molecule accepts the electron from ANBT, and the charge transfer of ANBT in the A orientation (AM1: −0.02 e, PM3: 0.01e, B3LYP/6-31G*:0.01e) is larger than in the B orientation (AM1: −0.01, PM3: 0.00 e, B3LYP/6-31G*: 0.00 e).

Table 4 lists the geometric parameters of ANBT before and after complexation in β-CD as obtained from AM1, PM3 and B3LYP/6-31G* calculations. It is evident that in β-CD (in both A and B orientations) the geometry of ANBT is completely altered. The alteration is significant in dihedral angles, which, indicates that ANBT must adapt a specific conformation to form a more stable inclusion complex.

4. Conclusion

In this study we confirmed by molecular modeling the inclusion process of the 3-amino-5-nitrobenzisothiazole in ß-cyclodextrin.

The stable structures and the inclusion process for ANBT/β-CD inclusion complexes were studied by use of force field MM+; quantum mechanics PM3 and AM1 methods.

From force field MM+ study, ANBT/β-CD inclusion complex in the A orientation was predicted to be the most stable structure. This result is completely similar to that obtained from semi-empirical PM3, AM1, single point HF and DFT calculations. The ANBT in the A orientation entered full in β-CD hydrophobic cavity, the NO2 group located near

Table 4
Geometrical parameters of ANBT before and after inclusion in β-CD, bond distances (Å), angle (°) and dihedral angles (°) calculated by AM1, PM3 and B3LYP/6-31G*methods.

	Free ANBT	A orientation	B orientation
	AM1/ PM3/B3LYP/6-31G*	AM1/ PM3/B3LYP/6-31G*	AM1/ PM3/B3LYP/6-31G*
Bond lengths (Å)			
S7-N9	1.64/1.73/1.79	1.64/1.73/1.73	1.46/1.73/1.73
N9-C10	1.34/1.33/1.29	1.34/1.33/1.33	1.34/1.33/1.33
C10-N11	1.39/1.40/1.35	1.38/1.39/1.36	1.39/1.40/1.36
C1-N8	1.48/1.40/1.44	1.48/1.49/1.42	1.48/1.50/1.50
N8-O12	1.20/1.49/1.32	1.20/1.22/1.23	1.20/1.22/1.19
N8-O13	1.20/1.21/1.22	1.20/1.21/1.19	1.20/1.21/1.21
S7-C4	1.68/1.21/1.79	1.68/1.73/1.73	1.68/1.74/1.71
Bond angles (°)			
C4-S7-N9	97.35/92.74/ 90.91	97.47/92.69/91.69	97.45/92.6594.64
S7-N9-C10	111.15/112.06/111.02	111.03/112.06/112.06	111.14/111.88/107.62
C10-N11-H17	115.75/114.46/118.54	117.04/115.09/115.09	115.85/114.88/120.50
C10-N11-H18	113.73/112.30/122.88	115.61/114.67/114.67	114.23/114.15/119.53
N9-C10-C3	113.39/114.12/116.92	113.32/114.19/114.10	113.39/114.62/117.14
C1-N8-O12	118.84/119.13118.16/	118.73/119.20/11919	118.67/118.90/121.06
C1-N8-O13	119.06/119.53/118.30	119.37/119.66/119.74	119.23/119.60/120.84
N9-C10-N11	125.09/120.67/120.75	125.01/119.66/119.62	125.00/118.98/119.64
Dihedral angle (°)			
C4-S7-N9-C10	1.32/−0.56/0.07	−1.17/−0.67/−0.67	1.47/0.90/1.26
S7-N9-C10-C3	−1.1.42/−20.58/0.03	1.43/0.93/ 0.93	−0.65/−1.47/0.20
N9-C10-N11-H17	13.44/0.77/0.00	−16.05/−18.54/−18.54	12.95/25.36/0.22
N9-C10-N11-H18	148.94/−151.30/−179.96	−157.93/−152.29/−6.44	148.43/158.40/153.56
C2-C1-N8-O12	1.38/−4.83/−0.09	5.42/−152.29/−6.44	−16.74/−16.9/−16.26
C2-C1-N8-O13	−178.77/175.31/− 1.79.96	−75.07/173.49/173.49	146.73/145.90/144.28

the primary hydroxyls and NH2 group near the secondary hydroxyls of β-CD is preferred according to the calculated energies.

In the two A and B orientations there is no interaction between the NH2 and NO2 groups of ANBT and the –OH groups of β-CD. This finding is in good agreement with experimental results. The driving forces governing the complexation process are mainly Van der Waals and hydrophobic interactions.

References

[1] S.H. Gellman, Chem. Rev. 97 (1997) 1231.
[2] R. Breslow, S.D. Dong, Chem. Rev. 98 (1998) 1997.
[3] J. Szejtli, Chem. Rev. 98 (1998) 1743.
[4] M.V. Rekharsky, Y. Inoue, Chem. Rev. 98 (1998) 1875.
[5] K.B. Lipkowitz, Chem. Rev. 98 (1998) 1829.
[6] S.K. Xing, C. Zhang, H.Q. Aib, Q. Zhaoa, Q. Zhang, D.Z. Sun, J. Mol. Liq. 146 (2009) 15–22.
[7] R. Breslow, Acc. Chem. Res. 28 (1995) 146.
[8] R. Breslow, Pure Appl. Chem. 70 (1998) 267.
[9] T. Loftsson, M.E. Brewster, J. Pharm. Sci. 85 (1996) 1017.
[10] F.C.G. Hoskin, D.M. Steeves, J.E. Walker, Biol. Bull. 197 (1999) 284.
[11] H.J. Schneider, F. Hacket, V. Rüdiger, H. Ikeda, Chem. Rev. 98 (1998) 1755.
[12] K. Harata, Chem. Rev. 98 (1998) 1803.
[13] L. Liu, X.S. Li, K.S. Song, Q.X. Guo, J. Mol. Struct. THEOCHEM 531 (2000) 127.
[14] L. Liu, Q.X. Guo, J. Incl. Phenom. Macrocycl. Chem. 50 (2004) 95.
[15] L. Liu, X.S. Li, T.W. Mu, Q.X. Guo, Monatsh. Chem. 131 (2000) 849.
[16] L. Liu, X.S. Li, Q.X. Guo, Y.C. Liu, Chin. Chem. Lett. 10 (1999) 1053.
[17] E.C. Yang, X.J. Zhao, F. Hua, J.K. Hao, J. Mol. Struct. 712 (2004) 75.
[18] C.L. Yan, X.H. Li, Z.L. Xiu, C. Hao, J. Mol. Struct. 764 (2006) 95.
[19] C.L. Yan, Z.L. Xiu, X.H. Li, C. Hao, J. Mol. Graph. Model. 26 (2007) 420.
[20] (a) H. Matsunaga, T. Matsui, K. Ohya, K. Okino, H. Hayashida, K. Maebayashi, N. Kiriika, D.J. Stein, Int. J. Psychiatry Clin. Prac. 10 (2006) 142;
(b) C. Branca, A. Torelli, M. Bass, Plant Cell Tissue Organ Cult. 21 (1990) 17.
[21] A.F. Brigas, C.S.C. Fonseca, R.A. Johnstone, J. Chem. Res. 2002 (2002) 299.
[22] P. Vicini, F. Zani, P. Cozzini, I. Doytchinova, Eur. J. Med. Chem. 37 (2002) 553.
[23] R. Rajamohan, S. Kothai Nayakib, M. Swaminathan, Spectrochim. Acta Part A 69 (2008) 371–377.
[24] Version 6.0, Cambridge software.
[25] L. Liu, X.S. Li, T.W. Mu, Q.X. Guo, Monatsh. Chem. 131 (2000) 849–855.
[26] W.J. Hehre, R. Ditchfield, J.A. Pople, J. Chem. Phys. 56 (1972) 2257–2261.
[27] Hyperchem, Release 7.51 for windows 2002 Hypercube. Inc.
[28] Gaussian 03, Revision B.01, M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, Jr., T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, and J.A. Pople, Gaussian, Inc., Pittsburgh, 2004.
[29] T.A. Halgren, J. Comput. Chem. 20 (1999) 730–748.
[30] A.D. Becke, J. Chem. Phys. 98 (1993) 5648–5652.
[31] C. Lee, W. Yang, R.G. Parr, Phys. Rev. B 37 (1988) 785–7899.
[32] M. Karelson, V.S. Lobanov, R. Katrizky, Chem. Rev. 96 (1996) 1027–1043.
[33] L. Liu, K.S. Song, X.S. Li, Q.X. Guo, J. Incl. Phenom. Macrocycl. Chem. 40 (2001) 35–39.