2013

Modelling bovine serum albumin inside carbon nanotubes

Ngamta Thamwattana
University of Wollongong, ngamta@uow.edu.au

Duangkamon Baowan
Mahidol University, University of Wollongong, db898@uow.edu.au

Barry J. Cox
University of Adelaide, University of Wollongong, barryc@uow.edu.au

Publication Details
Modelling bovine serum albumin inside carbon nanotubes

Abstract
Bovine serum albumin is commonly used in many biochemical applications due to its stability, lack of interference within biochemical reactions and low production cost. Here, we model the interaction of bovine serum albumin inside a carbon nanotube. The carbon nanotube is chosen as an example to demonstrate its potential use in targeted drug and protein delivery and as an enzyme immobilizing material. We consider three possible structures as models for bovine serum albumin which are cylinder, prolate ellipsoid and three-connected spheres. Using the Lennard-Jones potential together with a continuum approach we obtain explicitly analytical expressions for the interaction energies of each configuration inside a carbon nanotube. These expressions are employed to determine the critical size of a nanotube which maximises the interaction with each model structure of the bovine serum albumin. Knowledge of the critical size is important and may be crucial for the design of a nanotube for maximum loading of the proteins and drug molecules.

Keywords
modelling, inside, albumin, nanotubes, serum, carbon, bovine

Disciplines
Engineering | Science and Technology Studies

Publication Details

This journal article is available at Research Online: http://ro.uow.edu.au/eispapers/1679
Modelling bovine serum albumin inside carbon nanotubes

Ngamta Thamwattana,*a Duangkamon Baowanbc and Barry J. Coxd

Bovine serum albumin is commonly used in many biochemical applications due to its stability, lack of interference within biochemical reactions and low production cost. Here, we model the interaction of bovine serum albumin inside a carbon nanotube. The carbon nanotube is chosen as an example to demonstrate its potential use in targeted drug and protein delivery and as an enzyme immobilizing material. We consider three possible structures as models for bovine serum albumin which are cylinder, prolate ellipsoid and three-connected spheres. Using the Lennard-Jones potential together with a continuum approach we obtain explicitly analytical expressions for the interaction energies of each configuration inside a carbon nanotube. These expressions are employed to determine the critical size of a nanotube which maximises the interaction with each model structure of the bovine serum albumin. Knowledge of the critical size is important and may be crucial for the design of a nanotube for maximum loading of the proteins and drug molecules.

1 Introduction

Bovine serum albumin (BSA) is a globular protein, which is used in many biochemical applications due to its stability and lack of interference within biochemical reactions. Further, the production cost of BSA is relatively low compared to other proteins commonly used in laboratory, since large quantities can be readily purified from bovine blood, a byproduct from the cattle industry. BSA is generally used in enzyme-linked immunoassay (ELISA), immunoblots, and immunohistochemistry.1–7 ELISA provides a highly sensitive procedure for quantitating antigens and antibodies.1,2 BSA and protein Tween 20 are most often used to block vacant binding sites in ELISA.3 Immunoblotting (or western blotting) is a rapid and sensitive assay for the detection and characterization of proteins that works by exploiting the specificity inherent in antigen–antibody recognition.4,5 Immunohistochemical staining is a tool for detecting specific antigens in tissue.6,7 Further, BSA is applied to many laboratory molecular techniques, including restriction enzyme digestions of DNA to increase thermal stability and half-life of the restriction enzymes in the reactions.8 BSA is also commonly used to determine the quantity of other proteins, by comparing an unknown quantity of protein to known amounts of BSA.9 Also, BSA can further enhance the effects of organic solvents on increased yield of polymerase chain reaction of GC-rich templates.10 Lang11 finds that the H/anti-H reaction in routine ABO bloodstain grouping can be enhanced by incorporating a suitable amount of BSA.

In terms of the geometry and structure of BSA, a number of experiments reports the shape of BSA to be a prolate ellipsoid of revolution with the dimensions of 140 Å for the major axis and 40 Å for the minor axis (Fig. 1b).12,13 Other models for BSA...
include spherical subunit models which comprise one large sphere and two or three identical smaller spheres aligned in a linear chain.\textsuperscript{13,14} As an example, we only consider the subunit model that comprises three-connected spheres (Fig. 1(c)), noting that the mathematical formulation presented here can be easily extended to other spherical subunit models. The dimer of BSA is also studied through the subunit model of three-connected spheres.\textsuperscript{15} In this paper, following ref. 12–14 we examine typical models of BSA, namely the prolate ellipsoid and the three-connected spheres. Additionally, motivated by the long length of BSA we propose a new model here, which is the cylindrical structure (Fig. 1(a)). We note that the secondary structure of BSA mainly comprises $\alpha$-helix,\textsuperscript{15,16} and as such BSA may be viewed as a cylindrical tubular structure.

The present paper examines the scenario where BSA is assumed to be immobilized inside a carbon nanotube. In their study, enzymes are generally immobilized on a solid support to improve their stability.\textsuperscript{17} This immobilization of proteins and enzymes can prevent the rapid loss of biocatalytic effectiveness during the operation and storage periods resulting from autolysis effect, protein unfolding and aggregation. Among various nanomaterials (such as nanopores, nanofibers and nanotubes) carbon nanotubes are considered a promising material for enzyme immobilization research.\textsuperscript{18–20} According to ref. 18 and 19, immobilization of enzymes in a carbon nanotube can occur through noncovalent and covalent conjugations. Noncovalent attachment generally preserves the unique properties of both enzymes and carbon nanotubes, but the immobilized protein can leak and gradually disappear during the use of the nanotube–enzyme complex. Covalent conjugation provides durable attachment, but the enzyme structure may be more disrupted. The main goal is to create the stable attachment of enzymes that maintains as much as possible the activity and function of their native state. In this paper, we consider the noncovalent conjugation or the adsorption of BSA in carbon nanotubes. Since the immobilized enzymes prepared by adsorption tend to leak from the carriers, owing to the relatively weak interaction between the enzyme and the carrier,\textsuperscript{21} this paper predicts the critical size of carbon nanotubes which optimizes the interaction between BSA and a carbon nanotube, giving rise to the carbon nanotube–BSA complex that is most stable and minimises loss and leakage.

In addition to enzyme immobilization, carbon nanotubes represent a new class of molecular transporters that are potentially useful for \textit{in vitro} and \textit{in vivo} protein delivery applications.\textsuperscript{22,23} In particular, Kam \textit{et al.}\textsuperscript{22} show the intracellular transport of various types of proteins (streptavidin, protein A, BSA and cytochrome c) that are non-covalently and non-specifically bound to the sidewalls of single-walled carbon nanotubes. Furthermore, Ge \textit{et al.}\textsuperscript{24} find that the interaction of blood proteins (such as BSA, Tf, BFG and Ig) with single-walled carbon nanotubes can greatly alter their cellular interaction pathways which results in much reduced cytotoxicity for nanotubes coated with these proteins. Other studies such as ref. 25 and 26 also examine the adsorption/desorption of BSA on carbon nanotubes for biomedical applications. While ref. 22–26 concern the adsorption of BSA onto the external surface of the nanotubes, Kharlamova \textit{et al.}\textsuperscript{27} study the adsorption of BSA inside carbon nanotubes. We note that in ref. 27 the diameters of carbon nanotubes studied are quite large which are in the range of 20–180 nm and as such large amount of BSA molecules are able to adsorb at the internal surface of the carbon nanotubes. In this paper, we only examine the interaction of a single BSA molecule inside a carbon nanotube. We determine the dimension of the nanotube that allows the acceptance of the BSA molecule from rest and also the critical radius of the nanotube that gives rise to the most stable structure of BSA–carbon nanotube complex.

In the next section, we briefly introduce the Lennard-Jones potential and a continuum approach which are used to determine the interaction between BSA and carbon nanotubes. Also, in Section 2, we propose mathematical models for three possible configurations of BSA, which are cylinder, prolate ellipsoid and three-connected spheres. Numerical results are presented in Section 3 and a summary of the paper follows in Section 4.

### 2 Modelling approach

In this paper, we assume that the adsorption of BSA in carbon nanotubes is attributed to a process generally referred to as physical adsorption, or physisorption, mediated by van der Waals forces. To model the van der Waals interaction between BSA and a carbon nanotube we use the Lennard-Jones potential and a continuum approach. The Lennard-Jones potential is given by

$$\Phi(\rho) = -\frac{A}{\rho^6} + \frac{B}{\rho^{12}},$$

where $\rho$ denotes the distance between two atoms, $A$ and $B$ are the attractive and repulsive constants, respectively. For simplicity, we assume the isoelectric point (pH associated with zero net charge) for BSA,\textsuperscript{28} so that we may neglect the electrostatic energy in the present model. We comment that a system comprising carbon nanotubes and BSA considered here contains large amount of atoms. Thus, using molecular dynamics or atomistic modelling for this system would be computationally expensive. Through our approach we obtain analytical results, which is computational efficiency, even though we sacrifice some accuracy. However, we note in many areas the sacrifice is justified as the model captures the dominant interactions.

We model the interaction of BSA inside a carbon nanotube, where we consider three possible structures as models of BSA, which are a cylinder, a prolate ellipsoid and a chain of three-connected spheres, as shown in Fig. 1. The dimensions for each model are given in Table 1. Note that the dimensions for the ellipsoid and the spherical subunit models are obtained from ref. 12–14, whereas we assume the same radial and axial lengths to that of ellipsoid for the cylindrical model.

<table>
<thead>
<tr>
<th>Cylinder</th>
<th>$a = 20$ Å</th>
<th>$L = 70$ Å</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prolate ellipsoid\textsuperscript{12,13}</td>
<td>$a = 20$ Å</td>
<td>$b = 70$ Å</td>
</tr>
<tr>
<td>Three-connected spheres\textsuperscript{14}</td>
<td>$a = 26.6$ Å</td>
<td>$d = 19.0$ Å</td>
</tr>
</tbody>
</table>
Using a continuum approach, where atoms at discrete locations on the nanotube are averaged over its surface, the interaction energy between the atom at point P and the nanotube can be obtained by performing a surface integral of the Lennard-Jones potential over the nanotube, namely

\[ E_a = \eta_s \int_S \left( \frac{-A + B}{\rho^6} \right) dS = \eta_s (-AI_3 + BI_6), \tag{2} \]

where \( \eta_s \) represents the mean surface density of atoms on the nanotube. The integral \( I_n \) \((n = 3, 6)\) is defined by

\[ I_n = \int \rho^{-2n} dS. \tag{3} \]

Thus, from (1) and (3), we need to evaluate the following integrals

\[ I_n = c \int_{-\pi}^{\pi} \frac{1}{[(c - \delta)^2 + 4\delta c \cos^2(\theta/2) + z^2]} \, d\theta dz. \tag{4} \]

By introducing \( \lambda = \frac{(c - \delta)^2 + 4\delta c \sin^2(\theta/2)}{z^2} \) and substituting \( z = \lambda \tan \psi \) into (4) we obtain

\[ I_n = c \int_{-\pi/2}^{\pi/2} \cos^{2n-2} \psi \, d\psi \int_{-\lambda^{n-1}}^{\lambda^{n-1}} \frac{1}{\lambda^{n-1}} \, d\theta \]

\[ = c B(n - 1, 2, 1/2) \int_{-\lambda^{n-1}}^{\lambda^{n-1}} \frac{1}{\lambda^{n-1}} \, d\theta, \]

where \( B(x, y) \) denotes the beta function. Upon using \( t = \sin^2(\theta/2) \) yields

\[ I_n = \frac{2c}{(c - \delta)^{2n-1}} B(n - 1/2, 1/2) \int_{0}^{1} t^{1/2} (1 - t)^{-1/2} (1 - \mu t)^{1/2 - n} \, dt, \]

where \( \mu = -4\delta(c - \delta)^2\). The above integral is now in the Euler form, which from

\[ F(\alpha, \beta; \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma - \beta)} \int_{0}^{1} t^{\beta-1} (1 - t)^{\gamma-\beta-1} (1 - tz)^{-\alpha} \, dt, \]

we have

\[ I_n = \frac{2c}{(c - \delta)^{2n-1}} B(n - 1/2, 1/2) \frac{\Gamma(1/2)\Gamma(1/2)}{\Gamma(1)} F(n - 1/2, 1/2; 1; \mu) \]

\[ = \frac{2\pi c}{(c - \delta)^{2n-1}} B(n - 1, 2, 1/2) F(n - 1/2, 1/2; 1; \delta^2/c^2), \]

which gives

\[ I_n = \frac{2\pi c}{c^{2n-2}} B(n - 1, 2, 1/2) \sum_{m=0}^{\infty} \left( \frac{(n - 1/2)_m \delta^m}{m! c^m} \right)^2, \tag{5} \]

where \((a)_m\) is the Pochhammer symbol. By substituting (5) into (2) we obtain the interaction energy \( E_a \) between a carbon nanotube and an internal atom.

Next, we assume that the atom at point P is within the volume element of BSA. As such, we may determine the molecular interaction arising from the BSA by performing a volume integral of \( E_a \) over the volume of the protein, namely

\[ E_v = \eta_v \int E_a(\delta) \, dV = \eta_v \eta_s \int (-AI_3(\delta) + BI_6(\delta)) \, dV, \tag{6} \]

where \( I_n \) is given by (5), \( \delta \) is the distance from the nanotube axis to a typical volume element of the protein and \( \eta_v \) is the mean volume density of BSA, which depends on the assumed configuration of the protein. As such, we may write (6) as

\[ E_v = \eta_v \eta_s (-AK_3 + BK_6), \tag{7} \]

where the integral \( K_n \) is given by

\[ K_n = \int I_n(\delta) \, dV. \tag{8} \]
Based on (5), to find $K_n$ we need to evaluate the integral of the form

$$J_m = \int_0^\pi \int_0^\pi \int_0^1 a^{2m+2} b^{2m+2} \sin^{2m+1} \phi \, dr \, d\phi \, d\theta,$$

where $m$ is a nonnegative integer appearing in the summation from (5).

In the following subsections, we examine the three proposed model configurations for a BSA molecule, namely cylinder, prolate ellipsoid and three-connected spheres, and perform the volume integral (9) according to the geometry of each configuration.

### 2.1 Cylindrical model

Here we model the BSA as a cylinder centred at the origin with radius $a$ and length $2L$, as shown in Fig. 1(a). In a rectangular coordinate system, a typical point in the cylinder can be parameterized by $(ar \cos \theta, ar \sin \theta, z)$ where $0 \leq r \leq 1$, $-\pi \leq \theta \leq \pi$ and $-L \leq z \leq L$. Therefore, in this case the distance $\delta$ is given by $\delta^2 = a^2 r^2$, and the volume element is $dV = a^2 dr \, d\theta \, dz$. As a result, we have

$$J_m = \int_{-L}^{L} \int_{-\pi}^{\pi} \int_{0}^{a^2 r^2} dr \, d\theta \, dz = 4\pi La^{2m+2} \int_{0}^{1} t^{2m+1} dt = \frac{4\pi La^{2m+2}}{2m+2}.$$

On using a relation between a beta function and a gamma function, we have

$$J_m = \frac{2\pi La^{2m+2} m!}{(2)_m}.$$

Thus, from (5) and (8) find

$$K_n = \frac{8\pi^2 a^2 b}{3^{2n-2}} B(n-1/2, 1/2) \sum_{m=0}^{n} \frac{(n-1/2)_m(n-1/2)_m}{(5/2)_m m!} \left(\frac{a^2}{c^2}\right)^m.$$

Upon substituting (11) into (7), we may obtain the interaction energy of a cylindrical shaped BSA situated inside a carbon nanotube.

### 2.2 Prolate ellipsoidal model

Now we analyse a prolate spheroid with the axis of rotation collinear with the $z$-axis and centred at the origin. The equatorial semi-axes have length $a$ and the polar semi-axis (along the $z$-axis) has length $b$. The relation between the spheroidal and rectangular coordinates is given by

$$x = a \sin \phi \cos \theta, \quad y = a \sin \phi \sin \theta, \quad z = b r \cos \phi,$$

where $0 \leq r \leq 1$, $0 \leq \phi \leq \pi$ and $-\pi < \theta \leq \pi$. Then the offset distance $\delta$ is given by $\delta^2 = a^2 r^2 \sin^2 \phi$. Further, the volume element of the spheroid is $dV = a^2 b r^2 \sin \phi \, dr \, d\phi \, d\theta$. Hence, we may deduce

$$J_m = \int_{0}^{\pi} \int_{0}^{1} \int_{0}^{a^2 r^2} r^2 \sin \phi \, dr \, d\phi \, d\theta = 2\pi a^2 b \int_{0}^{\pi} \sin \phi \, d\phi \int_{0}^{a^2 r^2} dr = \frac{2\pi a^2 b (m+1)}{2m+3} B(m+1, 1/2).$$

Again on using a relation between a beta function and a gamma function, we have

$$J_m = \frac{4\pi a^2 b m!}{(2)_m}.$$

Thus, from (5) and (8) find

$$K_n = \frac{8\pi^2 a^2 b}{3^{2n-2}} B(n-1/2, 1/2) \sum_{m=0}^{n} \frac{(n-1/2)_m(n-1/2)_m}{(5/2)_m m!} \left(\frac{a^2}{c^2}\right)^m.$$

which upon substituting into (7), we can obtain the interaction energy of an ellipsoidal BSA inside a carbon nanotube.

### 2.3 Model of three-connected spheres

Here, we model BSA as a structure comprising three-connected spheres in a linear chain. We assume that the largest sphere has radius $a$ and that its centre is located at the origin. The two other spheres are assumed to locate on each side of the largest sphere and each has radius $d$. We note that we do not need to consider the interaction between each sphere here, since we assume that the molecule is at equilibrium.

To obtain the interaction energy for a sphere of radius $a$ inside a nanotube, we simply use the result from the previous section, whereby we substitute $b = a$ in the integral $K_n$ (14) to obtain

$$K_n = \frac{8\pi^2 a^3}{3^{2n-2}} B(n-1/2, 1/2) \sum_{m=0}^{n} \frac{(n-1/2)_m(n-1/2)_m}{(5/2)_m m!} \left(\frac{a^2}{c^2}\right)^m.$$

For the sphere of radius $d$, we may replace $a$ by $d$ in (15) to obtain $K_n$ which by substituting into (7) we can obtain the interaction energy for a sphere of radius $d$ inside a nanotube. As such the total energy for the BSA assuming to have the structure of three-connected spheres situated inside a carbon nanotube is given by

$$E_{\text{tot}} = E_a(a) + 2E_a(d).$$

### 3 Numerical results

In order to evaluate the interaction energy of a BSA inside a carbon nanotube, we need to determine the physical
parameters involved in the model. We note that there are 9684 atoms in a BSA molecule, comprising 3072 carbon, 4828 hydrogen, 816 nitrogen, 928 oxygen and 40 sulfur atoms. As a result we may determine the average attractive and repulsive constants between BSA interacting with a nanotube which is made up entirely of carbon atoms as

\[
A = (3072A_{CC} + 4828A_{HC} + 816A_{NC} + 928A_{OC} + 40A_{SC})/9684,
\]

\[
B = (3072B_{CC} + 4828B_{HC} + 816B_{NC} + 928B_{OC} + 40B_{SC})/9684,
\]

where \(A_{ij}\) and \(B_{ij}\) are the attractive and repulsive constants for atom \(i\) interacting with atom \(j\). Using the van der Waals diameters \(\sigma\) and well-depths \(\epsilon\) from Rappi et al.\(^{29}\) for each atom type and then employing the empirical combing rules \(\sigma_{ij} = (\sigma_i + \sigma_j)/2\) and \(\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}\), we find the attractive and repulsive constants from \(A_{ij} = 2\sigma_{ij}^6 \epsilon_{ij}\) and \(B_{ij} = \sigma_{ij}^{12} \epsilon_{ij}\) for the interaction between different type of atoms as shown in Table 2. As such, from (17) we obtain the values of \(A\) and \(B\) for BSA–carbon nanotube interaction as also given in Table 2. We note that the values of the van der Waals diameter and well-depth given in ref. 29 have been widely used in many research fields, including computational chemistry, physical chemistry and nanotechnology, and this work of Rappi et al. has been cited more than 1200 times.

We determine the atomic volume densities \(\eta_i\) for each configuration of BSA which can be found from dividing the total number of atoms in BSA by the volume of the assumed structure. For the cylinder model, \(\eta_a = 9684/(2\pi a^2 L)\). For the prolate ellipsoid, we have \(\eta_a = 9684/(4\pi a b)/3\). For the model of three-connected spheres, all the segments are assumed to be of equal density,\(^4\) and thus \(\eta_a = 9684/(4\pi a^3 + 2d^3)/3\). We note that the values for \(a, b, d\) and \(L\) for each configuration are given in Table 1. For the atomic surface density of a carbon nanotube, we use \(\eta_c = 0.3821 \text{ Å}^{-2}\) which is the same value to that of graphene.\(^{28}\) The numerical values for all of the atomic densities used in this paper are given in Table 3.

Using MAPLE, we plot the interaction energy for the three configurations of BSA situated inside a carbon nanotube. We assume that the carbon nanotube has radius \(c\) and is infinite in length. In Fig. 3 we plot for each configuration the relationship between the interaction energy and the radius of a carbon nanotube. From this figure, we observe a similar trend for all configurations. The equilibrium position for BSA lies a certain distance away from the inner surface of the nanotube where the interaction energy is minimum. The critical radius for the nanotube which minimises the interaction energy for each configuration is prescribed in Table 4. From Fig. 3 we can also deduce the minimum radius of a carbon nanotube that will accept each model configuration of BSA molecule from rest (see Table 5).

### Table 2 Numerical values of the attractive and repulsive constants

<table>
<thead>
<tr>
<th>Interaction</th>
<th>(A) (Å(^3) kcal mol(^{-1}))</th>
<th>(B) (Å(^{12}) kcal mol(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>C–C</td>
<td>684.9524</td>
<td>1 117 047.196</td>
</tr>
<tr>
<td>H–C</td>
<td>198.5959</td>
<td>145 063.9865</td>
</tr>
<tr>
<td>N–C</td>
<td>477.5906</td>
<td>669 934.5728</td>
</tr>
<tr>
<td>O–C</td>
<td>391.3802</td>
<td>482 466.7624</td>
</tr>
<tr>
<td>S–C</td>
<td>1274.868</td>
<td>2 395 472.866</td>
</tr>
<tr>
<td>BSA–carbon</td>
<td>399.3085</td>
<td>539 255.7407</td>
</tr>
</tbody>
</table>

### Table 3 Numerical values for various atomic densities

<table>
<thead>
<tr>
<th>Atomic density</th>
<th>(\eta) (Å(^{-2}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface density of carbon nanotubes</td>
<td>(\eta_c = 0.3812 \text{ Å}^{-2})</td>
</tr>
<tr>
<td>Volume density of cylindrical BSA</td>
<td>(\eta_a = 0.0550 \text{ Å}^{-3})</td>
</tr>
<tr>
<td>Volume density of ellipsoidal BSA</td>
<td>(\eta_a = 0.0826 \text{ Å}^{-3})</td>
</tr>
<tr>
<td>Volume density of each unit of spherical BSA</td>
<td>(\eta_a = 0.0710 \text{ Å}^{-3})</td>
</tr>
</tbody>
</table>

### Table 4 Critical radius of a carbon nanotube which optimizes the interaction with each model configuration of BSA

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Cylinder</th>
<th>Ellipsoid</th>
<th>Three spheres</th>
</tr>
</thead>
<tbody>
<tr>
<td>BSA</td>
<td>22.868</td>
<td>22.642</td>
<td>29.231</td>
</tr>
</tbody>
</table>

### Table 5 Minimum radius of a carbon nanotube which accepts each model configuration of BSA

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Cylinder</th>
<th>Ellipsoid</th>
<th>Three spheres</th>
</tr>
</thead>
<tbody>
<tr>
<td>BSA</td>
<td>22.385</td>
<td>22.156</td>
<td>28.742</td>
</tr>
</tbody>
</table>
ends of the cylinder require a slightly larger size of a carbon nanotube to accommodate the cylindrical BSA compared to that of the prolate ellipsoidal structure (see Table 4). For the model of three-connected spheres, the size of the nanotube is strongly dependent on the radius of the largest sphere. For all cases, we find that the shortest distances between the outer surface of the BSA and the inner surface of the nanotube are approximately 2.868, 2.642 and 2.631 Å for cylinder, prolate ellipsoid and three-connected spheres, respectively. We comment that the latter two models are more realistic as they are a closer match to the surface of a carbon nanotube. We note that this equilibrium is at equilibrium and most stabilized when the outer surface of BSA given in ref. 31 (i.e. a single sphere of radius 36 Å), where we find the critical radius of the nanotube to be 38.630 Å.

4 Summary

In this paper, we use the Lennard-Jones potential together with a continuum approach to model the interaction of a BSA molecule inside a carbon nanotube. Three model configurations of BSA are considered, which are cylinder, prolate ellipsoidal and three-connected spheres. We find that the cylinder has the maximum binding energy followed by the ellipsoid and the three-connected spheres. The maximum binding energy depends directly on the volume of the model configuration.

Inside a nanotube, BSA adopts an equilibrium location that is a certain distance away from the inner surface of the nanotube where the energy is minimised. The equilibrium distance between the BSA and the nanotube strongly depends on the radial dimension of the model configuration of BSA. For the case of three-connected spheres, the radius of the largest sphere strongly influences the critical size of the nanotube which gives rise to the optimal complex. In Table 4 we prescribe the critical radius of the carbon nanotube which optimizes the interaction energy for each configuration of BSA. We note that even though the cylinder and the ellipsoid have the same width at the centre of the molecule, the cylinder requires a larger radius nanotube to accommodate the molecule. This is likely due to the larger ends of the cylinder as compared to those of the prolate ellipsoid.

We comment that a knowledge of the critical radius of nanotube which optimizes the interaction with BSA is important for the design of materials for effective proteins and enzymes immobilization. In ref. 28, BSA and lysozyme are employed as model proteins to investigate the loading and release efficiencies of titania nanotubes for use in drug delivery. We comment that the mathematical formulation given here can be easily applied to investigate the interaction of BSA with titania nanotubes and other types of nanopores and channels.

Acknowledgements

The authors acknowledge financial support from the University of Wollongong (UOW) and UOW’s Internationalisation Linkage Grant Scheme. DB also acknowledges the Thailand Research Fund (TRG5680072).

References


