Journal of Molecular Liquids xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Interaction between DNA and cationic diester bonded Gemini surfactants

Zahid Yaseen [a,*], Sayeed Ur Rehman [b], Mohammad Tabish [b], Kabir-ud-Din [c]

[a] Department of Civil Engineering, Islamic University of Science and Technology, Awantipora, India
[b] Department of Biochemistry, Faculty of Life Sciences, Aligarh Muslim University, Aligarh 202002, India
[c] Department of Chemistry, Aligarh Muslim University, Aligarh 202002, India

ARTICLE INFO

Article history:
Received 15 March 2014
Received in revised form 7 May 2014
Accepted 21 May 2014
Available online xxxx

Keywords:
DNA–cationic Gemini surfactant interaction
Compaction of nucleotides
Molecular docking
Cationic diester bonded Gemini surfactants

ABSTRACT

The formation of the polyion-complex between three cationic diester bonded Gemini surfactants and DNA has been demonstrated systematically. This was studied through the electrostatic attraction between ammonium head groups of Gemini surfactants and the phosphate groups of DNA. Ethidium bromide exclusion assay indicates the interaction between DNA and diester bonded Gemini surfactants. DNA binding abilities with the Gemini surfactant depends on tail length which has been demonstrated by agarose gel electrophoresis and circular dichroism (CD) measurements. Dynamic light scattering measurements reveal that the ester bonded Gemini surfactants can induce the collapse of DNA into densely packed bead-like structures with smaller size. Molecular docking technique was also utilized to understand the mode and mechanism of interaction between DNA and the Gemini surfactants (pre-micellar form). In addition to electrostatic interactions between the negatively charged phosphate backbone of DNA and positively charged head groups of Gemini surfactants, self-association due to hydrophobic interactions between the alkyl tails of surfactant and the hydrogen bonding between the ester group of surfactant and nitrogenous bases, results in the compaction of nucleotides.

1. Introduction

The modern treatment protocol, known as gene therapy, is an approach to treat the inherited disease by transfection that is transferring a correct copy of the defective gene into the cells. In the field of bionanotechnology, nonviral gene delivery has been a goal for many years [1]. The inherent immunological risks with viral vectors provide large incentives towards the development of nonviral vectors capable of targeted and triggered release of DNA [2,3]. Various complex agents such as cationic surfactants, lipids, poly-electrolytes, multivalent ions and alcohols have been used in the development of new nonviral transfection agents for decades [4]. Earlier, *in vitro* and *in vivo* delivery of interferon-γ plasmid was achieved by using the m-s-m type model Gemini surfactants, the so-called alkanediyl-α,ω-bis(dimethylalkylammonium bromide), where m represents the carbon chain length of the alkyl tail and s the number of carbon atom in the spacer and the dependence of the carbon number (m) of the alkyl side chain and spacer on the transfection efficiency was determined [5]. Bhadani and Singh [6] reported the binding affinity of thioester spacers of imidazolium Gemini surfactants by agarose gel electrophoresis and ethidium bromide exclusion experiments. Despite remarkable progress of cationic surfactants in gene delivery, a number of limitations preclude enthusiasm including cytotoxicity, environmental concerns and aquatic toxicity which limit the practical usage of these surfactants [7]. Therefore, it is worthwhile to develop biodegradable, eco-friendly and biocompatible surfactants and study their interaction with DNA in aqueous solution in order to check their potential in gene delivery.

The architecture of surfactant plays vital role in controlling the interaction between DNA and surfactant. Incorporation of esters as the labile linker in variety of lipids results in successful transfection [8–10]. It has been shown that the orientation of the ester linkage can have significant effect on the transfection efficiency [11]. Cationic Gemini surfactants, structurally analogous to complex cationic lipids used for transfection studies, have received increasing attention as simpler models for transfection complexes [12–17]. An in-depth study of these systems could be beneficial for the better understanding of DNA–surfactant complex formation. The first important step for any agent to prove its transfection potential depends on its binding affinity, and mode of binding with DNA. Recently synthesized Gemini surfactants [18–20] (Scheme 1), containing cleavable diester group in the spacer part, referred to as m-E2-m type surfactant where m = 12, 14, and 16 is the number of carbon atoms in alkyl tail and E2 represents the diester group in the spacer part of Gemini surfactants (ethane-1,2-diyl bis(*N*,*N*-dimethyl-*N*-alkylammoniumacetoxy) dichloride) have special importance due to having two ester groups (E2). The surfactants m-E2-m have shown promising potential in solubilization of various polyaromatic carcinogenic materials [19,20]. These new diester-group-containing Gemini surfactants have low cmc (critical micelle concentration) values, with cleavable nature, and low cytotoxicity [19–21], which can be utilized in several technical areas including the biomedical application of gene delivery.

* Corresponding author. Tel.: +91 9797264038 (mobile).
E-mail address: zadn521@gmail.com (Z. Yaseen).

http://dx.doi.org/10.1016/j.molliq.2014.05.013
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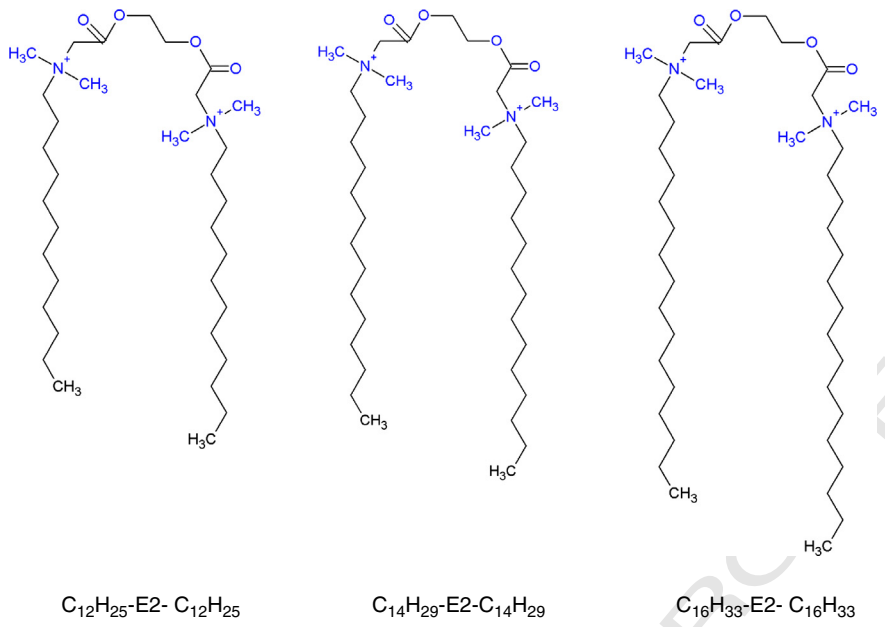


Scheme 1. Chemical structures of the ester bonded Gemini surfactants used in the present study.

In the present studies, we have investigated the interaction between dicationic ester bonded Gemini surfactants m-E2-m and DNA. The ultimate objective is to find out the mode of binding of these surfactants with DNA and also to relate the correlation between the alkyl tail length and DNA binding affinities. To achieve a deeper understanding of the interaction, a host of techniques have been employed to obtain broader and more integrated information. Based on these studies, we have shown herein that there exists a strong interaction between the diester-bonded Gemini surfactants and DNA. These studies reveal as how the hydrophobic effects and the specific surface charges play important roles in bringing about profound changes in DNA structures.

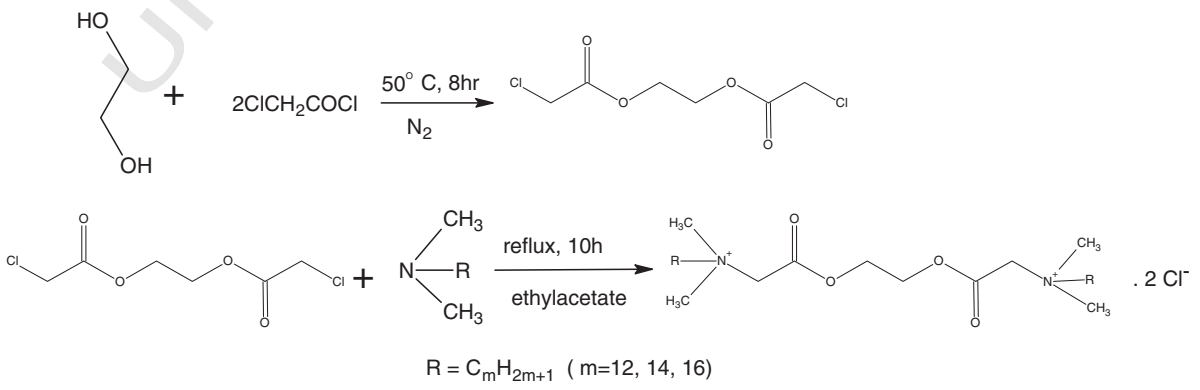
2. Experimental

2.1. Materials

Ethylene glycol, N, N-dimethylalkylamine, calf thymus DNA and ethidium bromide (EB) were purchased from Sigma Aldrich (St. Louis, USA). Plasmid pUC19 DNA (0.5 μg/μL, 2686 bp) was purchased from GeNei (India). Tris buffer was purchased from Fisher Scientific. The dimeric Gemini surfactants m-E2-m. $2Cl^-$ were synthesized by following a procedure described in the literature [18]. In brief, chloroacetyl chloride (0.22 mol) was added drop wise to ethylene glycol (0.1 mol) and the reaction mixture was heated at 50 °C for 8 h to obtain ethane-1,2-diylbis(chloroacetate). Ether was used in separation of ethane-1,2-diylbis(chloroacetate), followed by washing with saturated solution of sodium chloride. The organic phase was dried over magnesium sulfate. In the next step, a mixture of ethane-1,2-diylbis(chloroacetate) and N,N-dimethylalkylamine (molar ratio = 1:2.1) was refluxed for 10 h in ethyl acetate. Finally, the solvent was removed under vacuum and white crystalline solid of the cationic Gemini surfactants was obtained (Scheme 2). After recrystallization, the three surfactants were characterized by ^{1}H NMR and FT-IR [19–21]. The data were in agreement with the literature values. The purity was further ascertained on the basis of absence of minima in their surface tension–concentration isotherms [22].

2.2. Sample preparation

1 mg of calf thymus DNA was dissolved in 1 mL of 0.1 M Tris buffer (pH = 7.2) at 298 K and kept for 24 h with occasional stirring to ensure formation of a homogenous solution. The concentration of the DNA was determined spectrophotometrically using molar extinction coefficient of 6600 M^{-1} cm^{-1} at 260 nm [23]. The purity of the DNA solution was checked from the absorbance ratio A_{260}/A_{280}. Since the attenuance ratio of the above purified DNA lied in the range of $1.8 < A_{260}/A_{280} < 1.9$, no further purification was needed.



Scheme 2. Synthesis protocol of ethane-1,2-diyl bis(*N*,*N*-dimethyl-*N*-alkylammoniumacetoxy) dichloride Gemini surfactants.

Please cite this article as: Z. Yaseen, et al., J. Mol. Liq. (2014), http://dx.doi.org/10.1016/j.molliq.2014.05.013

2.3. Steady state fluorescence measurements

Fluorescence measurements were recorded on a Shimadzu spectrofluorimeter-5000 (Japan). In EB exclusion assay, the excitation with EB was set at 473 nm and emission in the range of 550–625 nm. 5 μg of pUC19 DNA in a volume of 10 μL was used for each experiment and DNA was directly mixed with 1 μL of EB in the fluorescence cell; buffer was added to make the final volume 3 mL.

2.4. Agarose gel electrophoresis

Different concentrations of surfactants, 3 μL of 0.5 μg/μL of pUC19 DNA and 2 μL of EB were mixed and incubated at room temperature for 1 h in a total volume of 10 μL. Samples were electrophoresed using 1% agarose gel and the DNA bands were visualized under UV transilluminator.

2.5. Circular dichroism measurements

Far UV-CD spectra were recorded on an applied Photo physics (U.K.) (model CIRASCAN) spectrophotometer equipped with a Peltier temperature controller using a rectangular quartz cuvette of path length 10 mm. The spectra shown are average of three successive scans recorded at a scan speed 200 nm/min. The contribution of buffer on the measured ellipticity was subtracted as blank. The data were subjected to noise reduction analysis. All the experiments were performed at ambient temperature (298 K) with air-equilibrated solutions and in Tris buffer of pH 7.0.

2.6. Dynamic light scattering measurements

Dynamic light scattering (DLS) measurements were performed using a Laser-Spectroscatter 201 by RiNA GmbH, Berlin, Germany. In DLS measurements, a beam of laser is guided towards the sample under investigation, with a fixed detection arrangement of 90° to the center of the cell area and the fluctuation in the intensity of the scattered light is measured. DNA and Gemini surfactant solutions were dissolved in Tris–HCl buffer and then mixed to obtain different DNA/surfactant molar ratios ([DNA] = 1 μM, [Gemini] = 0.2 to 5 μM).

2.7. Molecular docking

The rigid molecular docking studies were performed by using HEX 6.1 software [24], and PATCHDOCK [25]. HEX 6.1 is an interactive molecular graphics program for calculating and displaying feasible docking modes of DNA. The HEX 6.1 performs protein docking using Spherical Polar Fourier Correlations. It necessitates the ligand and the receptor as input in PDB format. The parameters used for docking include: correlation type — shape only, FFT mode — 3D, grid dimension — 0.6, receptor range — 180, ligand range — 180, twist range — 360, and distance range — 40. PATCHDOCK is an algorithm for molecular docking. The input is two molecules in PDB format and the output is a list of potential complexes sorted by shape complementary criteria. The crystal structure of the B DNA dodecamer d(CGCGAATTCGCG)$_2$ (PDB ID: 1BNA) was downloaded from the protein data bank. The initial structures of the surfactant molecules were generated by molecular modeling software Avogadro 1.01 using MMFF94 force field. The molecules of surfactants were optimized for use in the present docking study. They had their minimized total energy of 8.5–9.9 kcal mol^{-1}, respectively. Visualization of the docked pose has been done by using PyMol [26] (http://pymol.sourceforge.net/) molecular graphic or graphics program.

3. Results and discussion

3.1. Effect of Gemini surfactants on EB displacement assay

Ethidium bromide (EB) [27], a phenathridine fluorescence dye, is a typical indicator of intercalation that forms soluble complexes with nucleic acids and emits intense fluorescence in the presence of DNA due to the intercalation of the planar ring between the nucleotide base pairs of DNA. To study the interaction between DNA and other compounds, the changes in the spectra of EB on its binding to DNA are often used. Fig. 1 shows the fluorescence emission spectra of DNA/EB complex and the spectra after gradual addition of the Gemini surfactants. The progressive addition of surfactant into the premixed DNA–EB solution results in the displacement of intercalated EB from the DNA/EB complexes, leading to gradual fluorescence quenching. The concentrations of the surfactants (12-E2-12, 14-E2-14, 16-E2-16) required to displace ethidium bromide from the DNA, which brings decrease in fluorescence intensity, have been determined by plotting relative fluorescence intensity F/F_o, at 590 nm *vs.* concentration of surfactant (in mM), as shown in Fig. 1 (where F_o is the fluorescence intensity of DNA–EB complex and F is fluorescence intensity after adding surfactant to DNA–EB complex). It has been observed that quenching in fluorescence intensity is less in case of 12-E2-12; however, the behavior of decrease is almost similar in case of 14-E2-14 and 16-E2-16, though 14-E2-14 shows more quenching efficiency as compared to 16-E2-16. Increasing tail length of the surfactant results in an increase in hydrophobicity of the surfactant and, as a consequence, increased compaction efficiency. However, surfactants with too long chains may also provide sufficient amount of steric strains to get adjusted on the helical structure of DNA and also make the surfactant insoluble, therefore, be less efficient in DNA compaction [28].

The DNA–Gemini surfactant mixtures were made by mixing equal amount of pUC19 DNA with different concentrations of the Gemini surfactants and incubated for 60 min at room temperature. These mixtures were then subjected to electrophoresis after adding EB and the gel images were captured on UV transilluminator. As shown in Fig. 2 (lane a), pUC 19 DNA was run without any surfactant as control. The DNA + 12-E2-12 mixtures show noticeable fading of the bands and the band intensity shows consistent decrease with increasing concentration of the 12-E2-12 surfactant from 10 μM to 50 μM (lanes b–e).

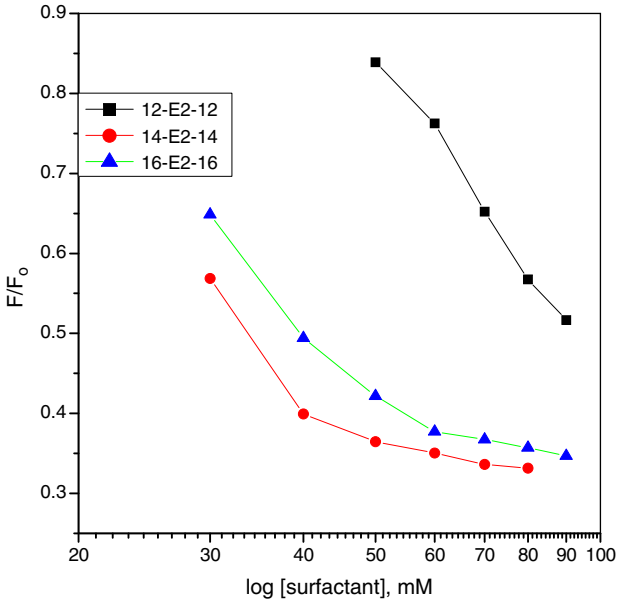


Fig. 1. Relative fluorescence intensity (F/F_o) observed at 590 nm *vs.* log concentration (mM) plot of DNA–EB-surfactant and DNA–EB complexes (λ_{exc} = 473 nm).

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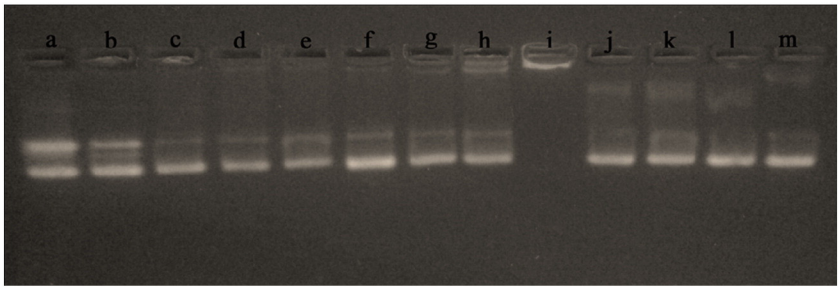


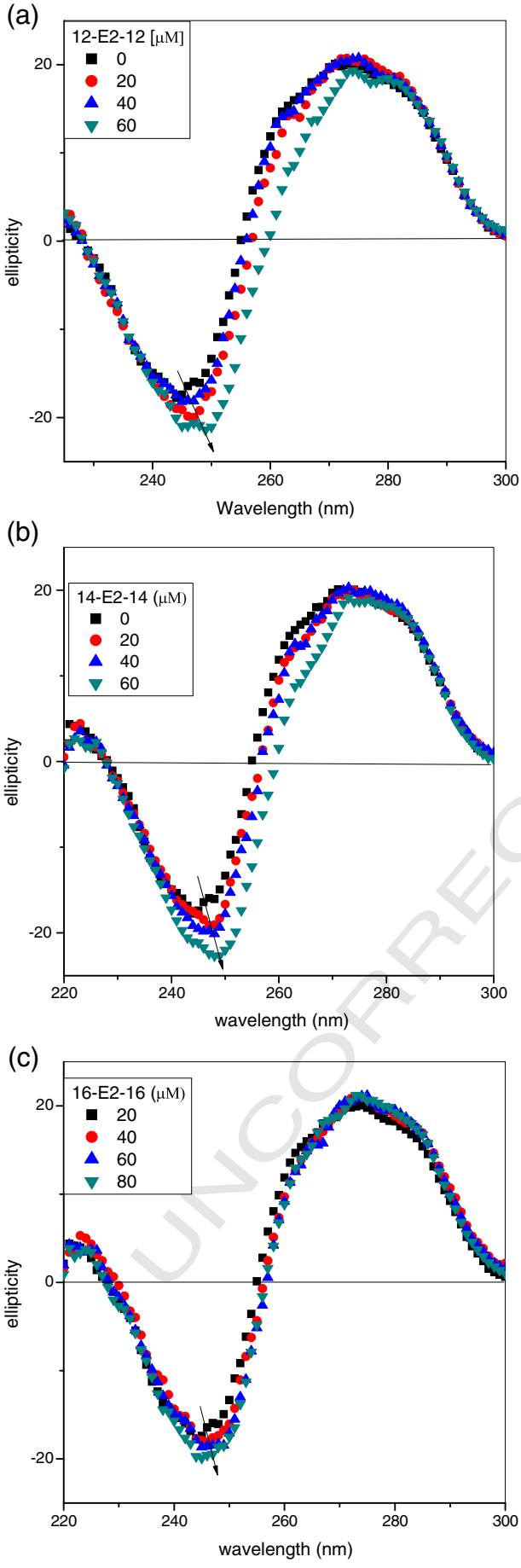
Fig. 2. Agarose gel electrophoresis of reaction mixtures containing DNA and cationic Gemini surfactants. The concentration of plasmid DNA was 150 ng/μL. (A) Lane a, DNA only; lanes b–e, DNA and 12-E2-12 (10, 20, 30, 50 μM); lanes f–i, DNA and 14-E2-14 (10, 20, 30, 50 μM); and lanes j–m, DNA and 16-E2-16 (10, 20, 30, 50 μM).

DNA + 16-E2-16 mixtures (Fig. 2, lanes j–k) also show slight reduction in the intensity of bands as compared to control and the band intensity decreases with increase in concentration of the surfactant. However, DNA + 14-E2-14 mixtures (Fig. 2, lanes f–i) display noticeable fading in the intensity of bands and there is almost complete disappearance of the DNA band at 50 μM of the surfactant. Thus, all the DNA–Gemini surfactant complexes exhibit a change in the intensity when compared with the control. The faint or invisibility of the DNA bands in the presence of Gemini surfactants in the agarose gel even after long ethidium bromide staining indicated that DNA–Gemini surfactant complexes lost the ability of intercalation towards the intercalator ethidium bromide. This may be assumed due to the compaction between DNA and Gemini surfactants. The DNA compaction may lead to alteration in the native structure of DNA in water. However, this form of DNA can still retain the double-stranded structure [29]. Such condensation of DNA leaves insufficient space available for ethidium bromide to intercalate and hence lose the fluorescence. The driving force for the compaction of DNA is electrostatic in nature, where positively charged head group of the surfactant interacts with negatively charged phosphate group of DNA. A possible explanation for the interaction between DNA and Gemini surfactants in concentration dependent manner is that the head group of Gemini surfactant itself experiences entropy loss due to electrostatic interactions with DNA. In order to compensate this loss, a large number of surfactant molecules have to be present to gain in hydrophobic interactions by self-association. This results in a highly compact DNA–Gemini surfactant complex and makes itself inaccessible to intercalators such as ethidium bromide.

To investigate the changes in the secondary structure of DNA upon binding with cationic Gemini surfactants, circular dichroism experiments were performed. This technique is useful to probe non-covalent DNA–ligand interactions [30,31]. The secondary structure of DNA is perturbed markedly by the intercalation of small molecules leaving its signature through the changes in the intrinsic CD spectra of DNA. Fig. 3 shows the CD spectra of DNA in buffer at pH 7, having a positive peak at ~277 nm and a negative peak at ~244 nm, characteristic of the right handed B form [32]. The peak position at 244 nm corresponds to the helical superstructures of the polynucleotide that provide an asymmetric environment for the nucleotide bases of DNA whereas peak at position 277 nm occurs due to stacking interaction between the bases of DNA. It is evident from Fig. 3 that there is noticeable change in the negative peak at 244 nm, with only a slight change in the intensity of the positive peak at 277 nm as the concentration of Gemini surfactants increased from 20 to 60 μM, indicating change in the conformation of DNA. Slight change in the intensity of the CD peak at 277 nm has been associated with alteration of hydration layer of the helix in the vicinity of phosphate or the ribose ring as the concentration of surfactant increased. On progressive addition of surfactants, the Tris (buffer) ions near the hydration layer of DNA helix may get exchanged with surfactant molecules. Hydrophobic alkyl chain of surfactants changes the extent of hydration near the phosphate group of DNA double helix and hence results in little perturbation in DNA helix. The peak at 244 nm becoming more negative with progressive addition of surfactants indicates the change in helicity of DNA double helix. This suggests that Gemini surfactant molecules get adsorbed on the surface of DNA and result in its compaction. It is evident from the Fig. 3 that the change in ellipticity of DNA double helix in presence of 14-E2-14 is more in comparison to 12-E2-12 and 16-E2-16, suggesting its stronger binding affinity with DNA.

3.2. DNA–surfactant interaction and hydrodynamic diameter

Dynamic light scattering (DLS) gives direct observation of the surfactant induced conformational changes in DNA chain, and size distribution of DNA/surfactant complexes could be obtained [33]. The variation in the hydrodynamic diameter as a function of the concentration of Gemini surfactant is shown in Fig. 4. DLS measurements could not be carried out for pure Gemini surfactants due to low scattering intensity. To avoid interaction between the DNA molecules, low concentration of DNA (1 μM) was used. A single peak in the intensity weighted size distribution of the DNA solution is attributed to the translational mode of the molecules and resulting in a mean hydrodynamic radius of about 300 nm. It was observed that with the addition of 0.2 μM of Gemini surfactant, there was a significant decrease in the size of DNA–Gemini complexes. As can be seen, with further addition of Gemini surfactants, a progressive decrease of the hydrodynamic diameter appears and finally becomes almost constant. Such an enormous decrease in the hydrodynamic diameter of the DNA–Gemini complexes indicates that the DNA undergoes a discrete conformational change from extended coiled state to a compact state by the addition of Gemini surfactants. The DNA molecule undergoes compaction that leads to a shift in the translational mode of DNA to lower hydrodynamic radius by the addition of surfactant molecules. Dias et al. [34] reported a gradual change of the DNA size in presence of CTAB (cetyltrimethyl ammonium bromide) and the existence of two populations in the sample, one of extended DNA coil coexisting with the DNA compacted molecules. However, in our case we have not found existence of two populations because of the abrupt change in hydrodynamic diameter of DNA, at very low surfactant concentrations. This may be attributed to the higher compaction efficiency of the ester bonded Gemini surfactants as compared to the conventional one head/one tail CTAB. Cationic surfactants interact with DNA by a combination of initial electrostatic interaction followed by a cooperative binding of surfactant ligands to the same DNA molecules (driven by hydrophobic forces). The diester group containing Gemini surfactants m-E2-m has cmc (critical micelle concentration) values in a range from 1.3 to 1.6 μM [19–21]. In the presence of a polyelectrolyte, surfactants show the aggregational behavior much below their cmc values. The compaction of DNA is depicted due to the surfactant self-assembly in the vicinity of the macromolecule; the surfactant self-assemblies are multivalent counterions which induce electrostatic attractions between different parts of a DNA molecule due to ion correlation effects [35,36]. In addition to this, ester bonded Gemini surfactants also have tendency to participate in hydrogen bonding between the oxygen atom of the ester group in the spacer part of Gemini



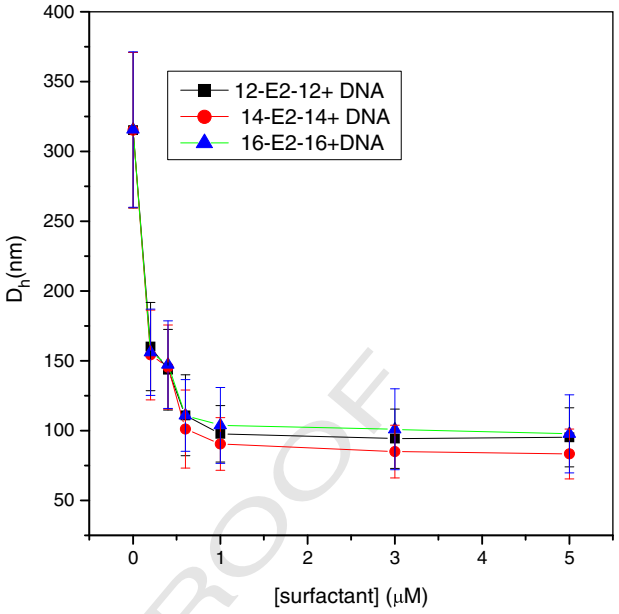


Fig. 4. Average hydrodynamic diameter D_h of DNA–Gemini surfactant complexes as a function of the surfactant concentration.

and the nitrogen bases in the nucleotide of DNA, leading to stronger interaction between the two components.

3.3. Computational analysis of DNA–surfactant interaction

Molecular docking technique is an attractive tool in order to understand the mechanistic details and mode of interaction between biopolymers and ligands, which can corroborate the experimental results. In this context docking studies were performed in an attempt to ascertain the type and the amount of interaction between the Gemini surfactants (in monomer form) and the DNA, as surfactant molecules bind to the polymer in pre-micellar region. In our experiments rigid molecular structure of DNA duplex with a sequence $d(CGCGAATTCGCG)_2$ dodecamer (PDB ID: 1BNA) was taken and the ligand has been made flexible to attain different conformations in order to predict the best fit orientation, and the best energy docked structure was analyzed. The docked structure, as shown in Fig. 5, suggests that the Gemini surfactants could bind to DNA by interacting with the phosphate backbone. The molecular-modeling predicted lowest energy conformation in which the head group of Gemini surfactant fits snugly into the curved contour of the targeted DNA in the minor groove and the tails of the surfactant molecules align themselves in parallel fashion to the DNA helix. Moreover, the ester groups of spacer part of the Gemini surfactants are situated near the Adenine ↔ Thymine region of DNA double helix. The ester groups in Gemini surfactant were stabilized by hydrogen bonding between the oxygen atoms and the hydrogen atoms of deoxy adenosine (DA5 and DA6 of strand A) of dodecamer. The resulting relative binding energy of docked DNA–Gemini surfactant complex was found to be ~ −160–180 kJ mol^{-1}, the negative values indicate higher binding potential of the Gemini surfactants with DNA. For comparison purpose, we have also run the docking program (HEX 6.1) on $C_{12}H_{25}N^+(CH_3)_3$. Br^-, monomeric analog of 12-E2-12, and the Gemini surfactant $C_{12}H_{25}N^+(CH_3)_2(CH_2)_8(CH_3)_2N^+C_{12}H_{25}\cdot 2Br^-$ and the energies evaluated were −114.2 and −140.11 kJ/mol, respectively. Thus more binding energies in case of m-E2-m surfactants with DNA give evidence of hydrogen bonding between the ester bonded Gemini

Fig. 3. Circular dichroism spectra of ct-DNA in presence of different concentrations of (a) 12-E2-12, (b) 14-E2-14, and (c) 16-E2-16 Gemini surfactants.

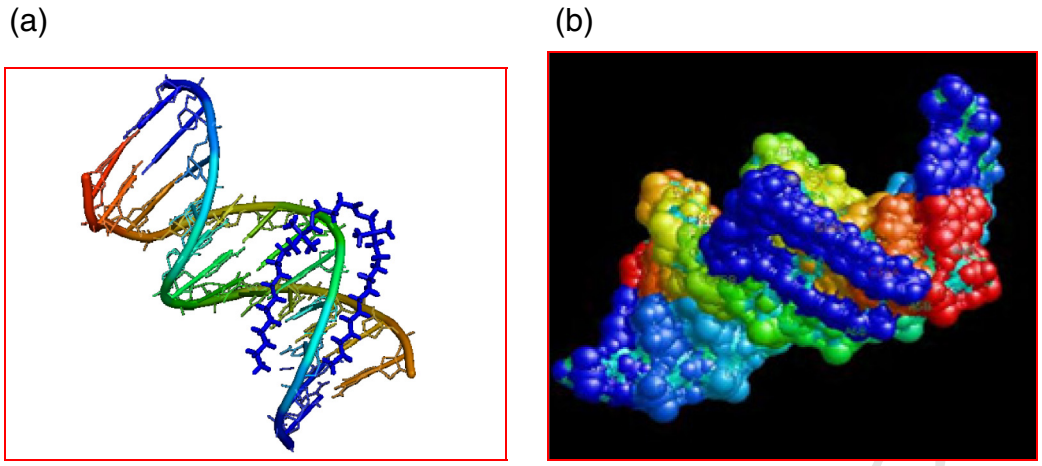


Fig. 5. Poses of molecular docked model of 12-E2-12 Gemini surfactant with DNA [dodecamer duplex of sequence d(CGCGAATTCGCG)$_2$ (PDB ID: 1BNA)].

surfactants and DNA. We see that there is a mutual complement between spectral techniques and molecular modeling, which provides valuable information about the mode of interaction of the Gemini surfactants with DNA.

4. Conclusions

The present work reports a study of the interaction of diester bonded cationic Gemini surfactants with DNA. Intercalation ability of ethidium bromide decreases in presence of the Gemini surfactants in ethidium bromide exclusion assay, which indicates the compaction potential of Gemini surfactants. This is also in agreement with the results obtained from gel electrophoresis. The outcome from circular dichroism measurements establishes that the Gemini surfactants interact with DNA in a groove binding fashion. These Gemini surfactants show chain length dependent binding capability as evidenced by fluorescence, electrophoresis and CD studies. The extent of interaction with DNA in case of 14-E2-14 is more as compared to 12-E2-12 and 16-E2-16. Due to the presence of positive charge on the head groups of Gemini surfactants, electrostatic binding of these self-organizing molecules to the anionic DNA phosphate is facilitated. Although the binding leads to entropy loss that is compensated due to hydrophobic interaction between the alkyl tails of surfactant, results in compaction of DNA are also revealed from DLS study. Large negative values of binding energy evaluated from molecular docking shed light on the possibility of hydrogen bonding also between the ester group of Gemini surfactants and nitrogenous bases of DNA.

Acknowledgements

KU thanks UGC, New Delhi, for the award of UGC-BSR Faculty Fellowship and Z Y acknowledges the UGC for awarding JRF. We also thank the Advanced Instrumentation Research Facility, Jawaharlal Nehru University (JNU), New Delhi, for helping us in carrying out the CD experiments.

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