Molecular Dynamics Study of the Interaction of GlyGluAsp Peptide Molecules with LysArgHis Dendrimer in Water

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Abstract: - Previously, it was shown that several short bioactive peptides, containing GluAsp (ED) sequence, can modulate gene expression and promote normalization of the function of different organs. In this work, we use Molecular dynamics simulations of the interaction between bioactive GlyGluAsp (GED) peptide molecules and a second-generation lysine dendrimer containing arginine-histidine (ArgHis) spacers. Unlike prior simulations involving charged double lysine or arginine (LysLys, ArgArg), neutral double hydrophobic (LeuLeu, AlaAla, GlyGly), and double pH-dependent (HisHis) spacers, this study focuses on dendrimers with HisArg spacers, where amino acids in the spacer are different, and histidine charge varies with pH. The simulation modeled the interaction of GlyGluAsp tripeptide and LysArgHis (KRH) dendrimer at two pH levels: (a) where histidine residues remain noncharged, and (b) where histidines are fully protonated. Results indicate that protonated histidines enable the dendrimer to carry a higher number of GED molecules, suggesting enhanced loading capacity at lower pH levels.

Key-Words: - Peptide dendrimers, oligopeptides, complexes, MD simulation, nanocontainer, drug delivery

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1 Introduction

Dendrimers are molecules distinguished by a regularly branched structure, setting them apart from traditional polymers [1]. Characterized by their monodispersity, spherical shape, high amount of reactive terminal groups, and internal cavities for hosting guest molecules, dendrimers offer versatile properties driven by their molecular architecture [2]. A combination of these properties made them very attractive for application in biomedicine and industry [3], [4]. They have multiple applications as vehicles for drugs [5], [6] or genetic material [7]. Dendrimers increase drug solubility. Application of several specific dendrimers for gene transfection was demonstrated in [7], in particular for transfection of DNA in [8], and for transfection of siRNA in [9] and [10]. Novel dendrimers were described recently in [11], internally functionalized dendrimers in [12], and various types of new dendrimers in [13]. A general overview of applications of new highly branched molecules for drug delivery was made in [14], and across blood brain barrier in [15]. Dendrimers for cancer therapy were reviewed in [16], for brain targeting in [17], and for gene therapy in [18]. New carbosilane dendrimers with PEG and positively charged end groups for siRNA transfection [19] and silencing of SARS-CoV-2 in [20] were also. But peptide dendrimers could work better than synthetic dendrimers in biomedicine. The first

aminoacid-based dendrimers contained only lysine residues [21]. These dendrimers were investigated in dimethylformamide for generations G=1-10 [22] and in water for G=3, [23] and for G=1-5, [24], [25], [26] for G=1-6 with modified end groups, [27]. NMR relaxation in similar dendrimers was studied also, [28], [29]. Multiple antigen peptides based on these dendrimers with terminally attached linear peptides were introduced in [30] and [31]. Incorporation of aminoacid residues inside lysine dendrimer was suggested in [24] and [32]. Dendrimers G=4 with additional arginine and lysine terminal residues were investigated in [33]. Dendrimers of generation 5 or 6 with arginine ends were introduced in [34]. Polyethyleneimine (PEI) dendrimers with arginine/lysine/leucine insertions were investigated in [35]. Results for similar dendrimers of G=6 with histidine/arginine terminal residues were obtained in [36]. PAMAM with G=4 having histidine/arginine ends were investigated in [37]. Branched polyglycerol amines with arginine/histidine terminal groups were discussed in [38] and [39] and lysine-based dendrimers with double glycine/lysine, [40], arginine, [41] and histidine [42] were studied also. Last stimuli-responsive dendrimers could be used for controlled encapsulation and release of drugs. In this paper, we study complexes made of similar pH dependent dendrimers and molecules of stress-protective tripeptides GED. These dendrimer complexes aim to shield the peptides from the digestive environment, enhancing their stability during delivery and bioavailability.

2 Model and Method

Molecular dynamics simulations were conducted for a system containing one LysArgHis (KRH) dendrimer, structured as a second-generation lysine dendrimer with an AlaLys (AK) core, LysArgHis (KRH) repeating units, and positively charged terminal Lys (K) residues with NH3+ groups. This setup included 16 molecules of GlyGluAsp (GED) tripeptide molecules, in water solvent, with counterions in a cubic simulation cell under periodic boundary conditions. We used equilibrated dendrimer conformations obtained from a previous simulation of the same dendrimers in water (without tripeptides). Tripeptide molecules in b-sheet initial conformation were obtained using Avogadro molecular editor. For the initial minimization of the energy and subsequent MD simulation, the GROMACS software and the Amber force field (AMBER_99SB-ildn) were used [43]. This force field calculates potential energy components, including valence bond potential, bond angles potential, dihedral angle potential, van der Waals potential, and electrostatic potential. Electrostatic interactions were managed through the Particle Mesh Ewald approach. All calculations were done in the NPT ensemble at normal conditions (pressure 1 atm and temperature 300 K) during total time equal 500 ns under two distinct pH conditions: first one at pH > 7, where histidine residues (His or H) of LysArgHis (KRH) dendrimer remain neutral, and second at pH < 5, where histidine residues of LysArgHisp (KRHp) dendrimer are fully protonated (Hisp or Hp) with a charge of +1. For the analysis of MD trajectories, we applied functions, algorithms, and programs previously developed for studying the properties of neutral, [44], [45] and charged linear [46], [47], and branched, [48], macromolecules as well as for polymer brushes, [49], [50].

3 Results and Discussion

Complex formation. To evaluate the complex formation process, the distance (*d*) function between peptides and dendrimer was calculated over time (see Figure 1). At the initial moment, the distance between the peptides and dendrimers is large, since the peptides are far from the center of mass of the dendrimer. After that, the distance decreases sharply during the first 50-100 ns and goes to a plateau value where it fluctuates around the average value. The plateau values of distance *d* look similar for both KRH and KRHp dendrimers. It is worth noting that the oscillations are more pronounced in the system with a dendrimer with uncharged inserts (Figure 2a) because for this less charged dendrimer (with neutral histidines in spacers), the electrostatic repulsion between charged groups is weaker.

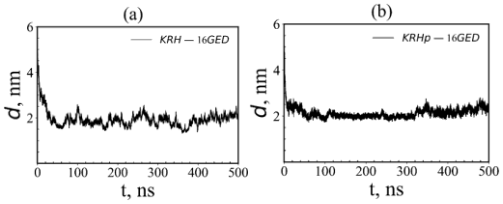

Fig. 1. Instant distance (*d)* from the centres of mass of the GED peptide molecules to the centres of mass of the (a) KRH or (b) KRHp dendrimers vs time (t). Source: created by the authors.

The instantaneous count of the number of peptide molecules forming a complex with the dendrimer was calculated as shown in Figure 2. To determine if a molecule remained within the dendrimer complex, we applied local criteria. We set a local parameter s = 1.5 and used it to multiply the sum of the van der Waals radii of the closest atoms of the dendrimer and each peptide molecule. If the distance *d* between

these atoms satisfied the condition $d <$ (sum of vdW radii) × s, the peptide was considered in contact (i.e. in complex) with the dendrimer. The calculated values of the number of peptide molecules N in complex (Figure 2) go to a plateau after 50–100 ns, indicating stable complex formation for both KRH dendrimer (Figure 2a) with neutral histidines (H) and for KRHp dendrimer (Figure 2b) with protonated histidines (Hp). It is easy to see from these plots that the plateau value of the number of GED peptides in the complex is greater for the KRHp dendrimer than for the KRH dendrimer.

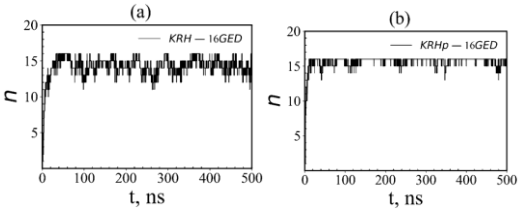

Fig. 2. Instant number of peptides (*n)* in complexes of (a) KRH and (b) KRHp dendrimers with GED peptide molecules vs time t. Source: created by the authors.

Equilibrium characteristics. To characterize the shape of the dendrimer and the complex, we used the asphericity parameter. It was found that this value is very close to zero for all systems. This means that the shape of both the dendrimer and the complex is very close to spherical. Thus, the structure of the dendrimer and peptide molecules in the complex can be described by the radial density distribution of their atoms around the dendrimer center of mass (Figure 3). This distribution reveals that dendrimer atoms (middle curve) are concentrated predominantly at the complex center, near r = 0. Peptide atoms (lower curve), meanwhile, show significant penetration into the dendrimer's interior, particularly in the KRHp dendrimer compared to KRH (as indicated by Figure 3b compared to Figure 3a). The combined atom density for all atoms of complex (upper curve) is a sum of density of dendrimer atoms (middle curve) and peptide atoms (lower curve), illustrating the spatial arrangement within the complex.

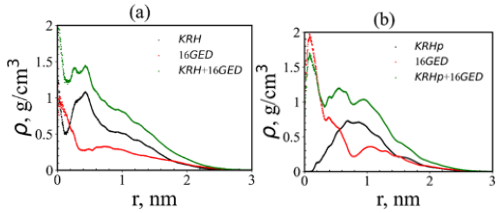

Fig. 3. Density profile ρ(r) for complexes of (a) KRH dendrimer and (b) KRHp with 16GED peptide vs radial distance (r) between them. Source: created by the authors.

From Figure 3 it is easy to see that the peptide molecules penetrate better (density about 2 g/cm3 at r=0nm) into the more charged KRHp dendrimers (with protonated histidines (Hp) in the dendrimer spacers) compared to KRH where density of GED atoms also has maximum at r=0 but the density is twice lower and close to 1 g/cm3). Thus, the atoms of GED peptides displace the KRH (Figure 3a) and KRHp (Figure 3b) dendrimer atoms from the center of the complex, but this displacement is more pronounced for the KRHp dendrimer with a higher charge.

Table 1. The mean distances (<*d*>) from each peptide to dendrimer, the mean amount of hydrogen bonds (<n_{HB}>) between peptides and dendrimers, the mean quantity of peptides (<*N*>*)* in the complex. Source: created by the authors.

System	<*d*>	<n_{Hb}>	<*N*>
KRH +16GED	1.90	56	14.2
KRHp+16GED	2.15	51	15.9

Mean values in Table 1 summarize the average structural characteristics of the studied complexes: the mean distance between GED molecules and dendrimer, the number of hydrogen bonds between them, the overall size of the complexes, and the number of GED molecules in it. These average values are consistent with the trends observed in Figure 1, Figure 2, and Figure 3. Thus, all mean values are in good agreement with the results obtained in the previous part of the paper.

4 Conclusion

We carried out MD calculations to investigate the interactions of molecules of GED tripeptide with second-generation lysine dendrimers KRH (with neutral histidines) and KRHp (with protonated histidines). We obtained that the dendrimer with protonated histidines forms complexes containing a greater number of GED tetrapeptide molecules than nonprotonated ones. We also demonstrated that GED tripeptide molecules penetrate deeper into the dendrimer. In the near future we plan to make synthesis, experimental study and simulation of new peptide dendrimers and their interactions with various food peptides [51].

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Contribution of Individual Authors to the Creation of a Scientific Article (Ghostwriting Policy)

The authors equally contributed in the present research, at all stages from the formulation of the problem to the final findings and solution.

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Conflict of Interest

The authors have no conflicts of interest to declare that are relevant to the content of this article.