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Bioinorganic Membrane Using Kurumi, A New Liquid Crystal

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Abstract

The work characterizes develop a single layer bioinorganic membrane using nano-molecule Kurumi $C_{13}H_{20}BeLi_2SeSi$ / $C_{13}H_{19}BeLi2SeSi$, is well characterize computationally. As its scientific name 3-lithio-3-(6-{3-selena-8-beryllatricyclo [3.2.1.0^{2},^{4}]oct-6-en-2-yl}hexyl)-1-sila-2-lithacyclopropane. The work was based on a molecular dynamics (MD) of 1ns, using the CHARMM22 force field, with step 0.001 ps. Calculations indicate that the final structure, arrangement have the tendency to form a single layer micellar structure, when molecular dynamics is performed with a single layer. However, when molecular dynamics were carried out in several layers, indicates the behavior of a liotropic nematic liquid crystal order. Kurumi features the structure polar-apolar-polar predominant. Limitations our study has so far been limited to computational simulation via quantum mechanics e molecular mechanics (QM/MM), an applied theory. Our results and calculations are compatible and with the theory of QM/MM, but their physical experimental verification depend on advanced techniques for their synthesis, obtaining laboratory for experimental biochemical. Going beyond imagination, the most innovative and challenging proposal of the work advances the construction of a structure compatible with the formation of a "new DNA", based now on the kurumi molecule.

Keywords: Membrane; Kurumi; Liquid Crystal; DNA; QM/MM; Hydrophobic; Hydrophilic; Single layer; Micellar; Structure; Biomembrane; Polar; Apolar.

1. Introduction

The work characterizes develop a single layer bioinorganic membrane using nano-molecule Kurumi $C_{13}H_{20}BeLi_2SeSi$ / $C_{13}H_{19}BeLi2SeSi$, is well characterize computationally. As its scientific name 3-lithio-3-(6-{3-selena-8-beryllatricyclo[3.2.1.0^{2},^{4}]oct-6-en-2-yl}hexyl)-1-sila-2-lithacyclopropane [1-8].

Getting Kurumi name [8], which means boy in Tupi-Guarani language, which are indigenous inhabitants of southern Brazil.

The Raman spectrum was calculated, indicating the characteristic of the bioinorganic nano-molecule genesis. Now the challenge is to build the basic structure of the bio-inorganic membrane [6].

The kurumi seed molecule has been well characterized, [1-9] and is in accordance with the *ab initio* computational methods [10-14]. Now the challenge is to build the basic structure of the bioinorganic membrane. The study evolved to construct a biomembrane from the seed molecule (kurumi) [1-8]. The calculations default already performed admit a hydrophobic and hydrophilic molecule, the basis of the formation of a micelle and or biomembrane, as the default template [9].

But kurumi molecule is polar-apolar-polar characteristic is predominant, ie. a hydrophilic-hydrophobic-hydrophilic molecule, thus presenting another standard for the construction of a biomembrane, which is even more innovative because a bioinorganic molecule [1-8].

Preliminary bibliographic studies did not reveal any works with characteristics studied here, except the works of the authors [1-9].

2. Methods

The software used for MD's outside the Program, with the CHARMM22 [15, 16] force field, in addition to HyperChem 8.0.6 Evaluation [17].

The computer used for MD was a Desktop with SUSE Linux Enterprise Desktop, AMD Ryzen 7 1800X processor, ASUS Prime A320M-K motherboard, 16GB of RAM, with 500GB SSD [18]

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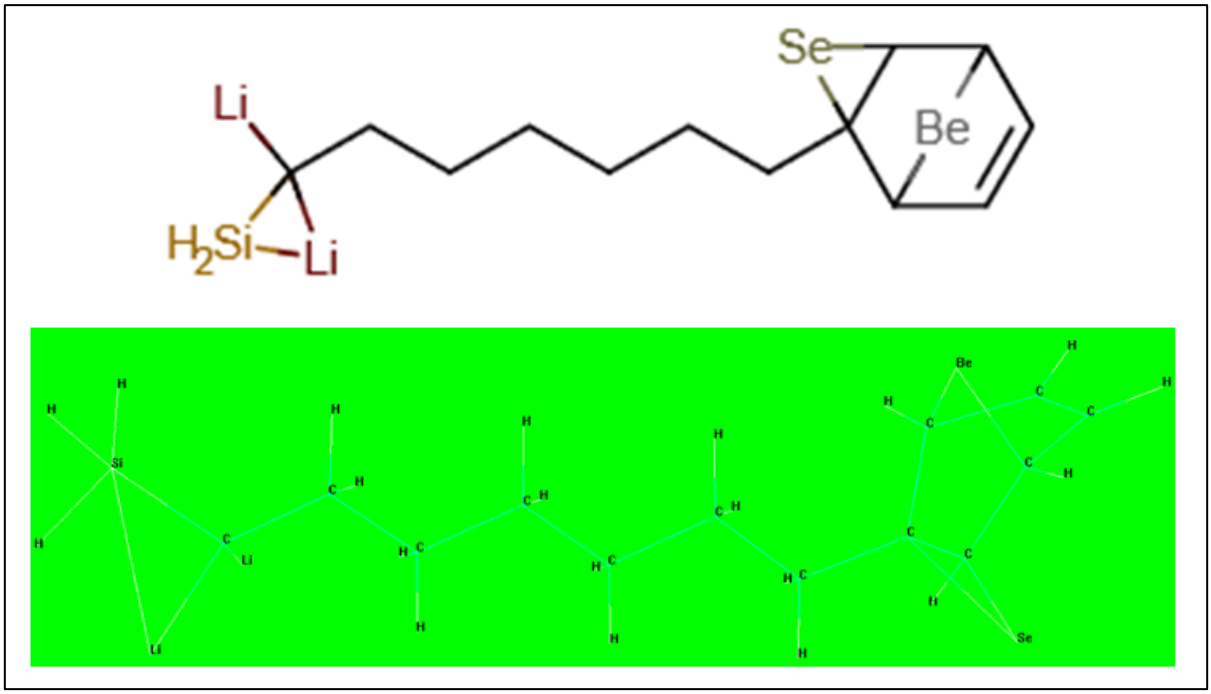
Figure-1. Representation of the molecular structure of $C_{13}H_{19}BeLi_2SeSi$, Nano-molecule Kurumi, 3-lithio-3-(6-{3-selena-8-beryllatricyclo[3.2.1.0²,⁴]oct-6-en-2-yl}hexyl)-1-sila-2-lithacyclopropane, obtained through computer via *ab initio* calculation method RHF/CC-pVTZ. [8, Authors]



3. Arguments and Results

The Figure (1) representation of the molecular structure of $C_{13}H_{20}BeLi_2SeSi$ / $C_{13}H_{19}BeLi_2SeSi$, Nano-molecule Kurumi,3-lithio-3-(6-{3-selena-8-beryllatricyclo[3.2.1.0²,⁴]oct-6-en-2-yl}hexyl)- 1-sila-2- lithacyclopropane. [8, Authors]

The Figure (2) represents results of MD, in a cubic box with water, dimensions 25 x 25 x 41Å, with 40 Kurumi molecules, 1031 water molecules, (the water molecules were removed to facilitate visualization) structural dimensions for a 10 x 4 x 1 Kurumi arrangement, 300K temperature, the final structure indicates the tendency to form a single layer micellar [19, 20] structure.

The Figure (3) represents results of MD in a cubic box with water, dimensions 40 x 30 x 56,1041Å, with 192 Kurumi molecules, 1353 water molecules, structural dimensions for a 12 x 4 x 4 Kurumi arrangement, temperature of 300K, the final structure indicates the formation of a nematic [19, 20] arrangement of liquid crystal.

The final structure indicates the tendency to form a single layer micellar structure, when MD is performed with a single layer. However, when molecular dynamics were carried out in several layers, indicates the behavior of a liotropic nematic [19-21] liquid crystal order.

Kurumi features the structure polar-apolar-polar predominant [21]. The orientational order of the Kurumi molecule in the micelle has the aromatic ring on the outside and the tail end with silicon and internal lithium.

4. Conclusion

With initial MD, in a cubic box with water, dimensions 25 x 25 x 41Å, with 40 Kurumi molecules, 1031 water molecules, structural dimensions for a 10 x 4 x 1 Kurumi arrangement, with outer radius 15Å, inner radius 11Å, 300K temperature, the final structure indicates the tendency to form a single layer micellar structure. Also form a single layer micellar structure with initial MD, in a cubic box with water, dimensions 56,1041 x 30 x 56,1041Å, with 144 Kurumi molecules, 1624 water molecules, structural dimensions for a 12 x 12 x 1 Kurumi arrangement, with outer radius 15Å, inner radius 1Å , temperature of 300K.

With initial MD, in a cubic box with water, dimensions 40 x 30 x 56,1041Å, with 192 Kurumi molecules, 1353 water molecules, structural dimensions for a 12 x 4 x 4 Kurumi arrangement, with outer radius 15Å, inner radius 11Å, temperature of 300K, the final structure indicates the formation of a nematic arrangement of liquid crystal.

The final structure indicates the tendency to form a single layer micellar structure, when MD is performed with a single layer. However, when molecular dynamics were carried out in several layers, indicates the behavior of a liotropic nematic liquid crystal order.

The orientational order of the Kurumi molecule in the micelle has the aromatic ring on the outside and the tail end with silicon and internal lithium.

Going beyond imagination, the most innovative and challenging proposal of the work advances the construction of a structure compatible with the formation of a “new DNA”, based now on the seed molecule.

Limitations our study has so far been limited to computational simulation via quantum mechanics e molecular mechanics (QM/MM), an applied theory. Our results and calculations are compatible and with the theory of QM/MM, but their physical experimental verification depend on advanced techniques for their synthesis, obtaining laboratory for experimental biochemical.

Figure-2. Represents results of MD, in a cubic box with water, dimensions 25 x 25 x 41Å, with 40 Kurumi molecules, structural dimensions for a 10 x 4 x 1 Kurumi arrangement, 300K temperature, the final structure indicates the tendency to form a single layer micellar structure. [Authors]

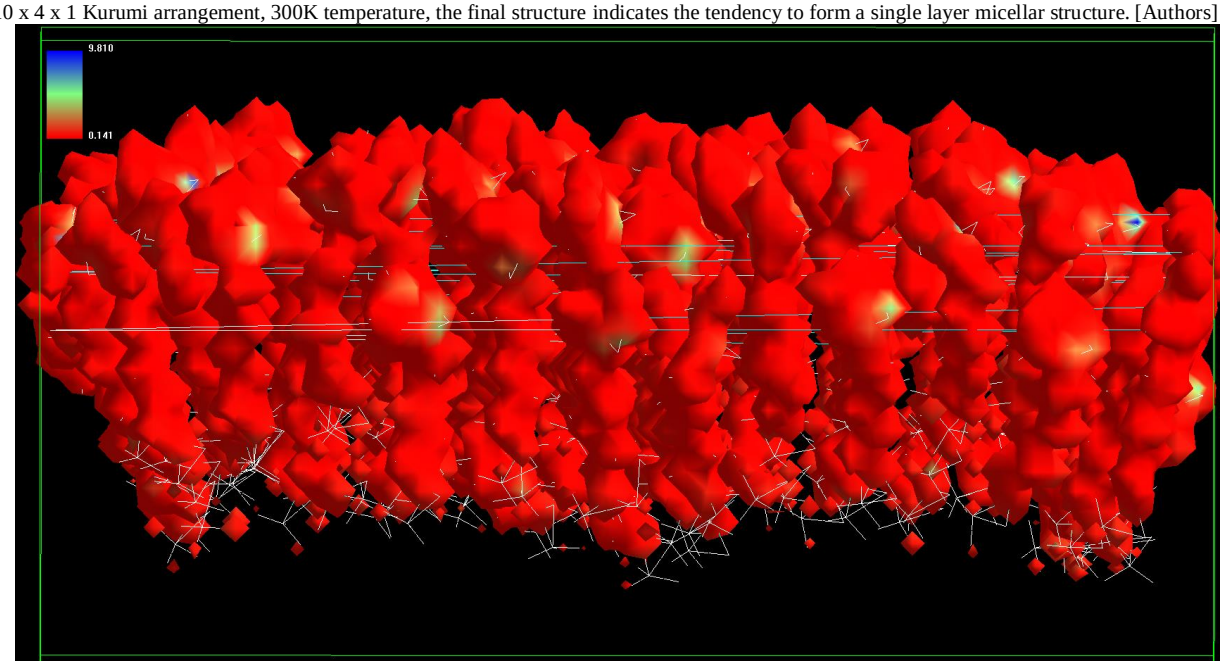
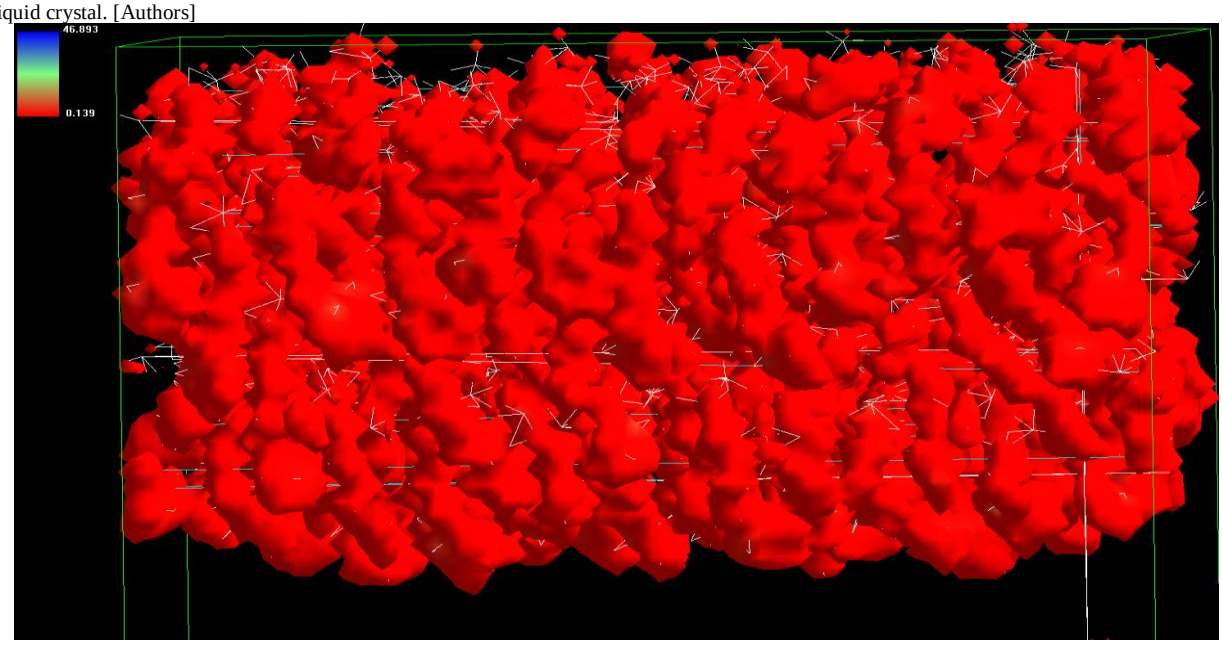


Figure-3. Represents results of MD in a cubic box with water, dimensions 40 x 30 x 56,1041Å, with 192 Kurumi molecules, structural dimensions for a 12 x 4 x 4 Kurumi arrangement, temperature of 300K, the final structure indicates the formation of a nematic arrangement of liquid crystal. [Authors]



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