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Virtual Reality Visualization For Complex Protein Structures Using Nanome

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Introduction

Nanome is a Virtual Reality based application allowing users to visualize and interact with chemical compounds/molecules and communicate with set virtual communities. With the help of Nanome, different user groups can gain different levels of insight from their experience. As a blend of science and technology, Nanome not only allows users to "walk into science," it also provides us with a prototype of the future metaverse classroom.

Key Findings

The immersive VR capabilities allow users to interact with data in a more intuitive and immersive way, making it easier to spot patterns and relationships that may not be immediately apparent in 2D renderings. The customized plugin in this research allows users to visualize and analyze the connectivity between atoms in molecular structures. This can users understand chemical interactions and identify potential drug targets or design new molecules.

Methods

Base Algorithm:
The base algorithm used in this plugin is the Depth-First Search (DFS) algorithm, which is a well-known algorithm used in graph traversal. In this algorithm, a starting node is chosen and visited, and then its neighboring nodes are visited recursively until all the nodes in the graph have been visited.

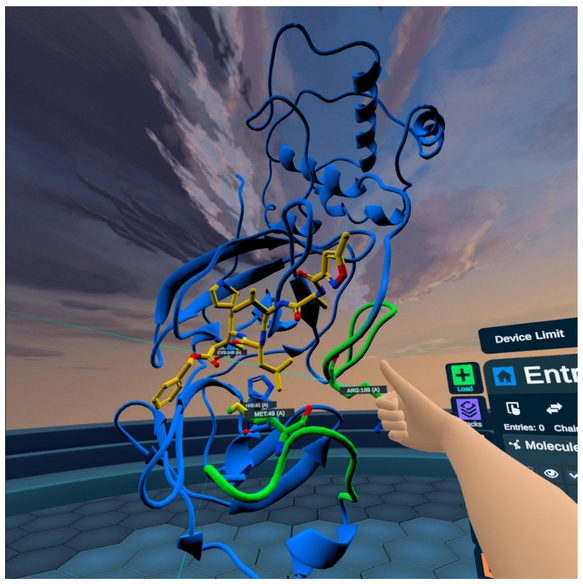
Customized Plug-In:
In the context of the plugin, the graph represents a molecule, where the atoms are nodes, and the bonds between them are edges. The DFS algorithm is used to traverse the graph and find all atoms connected to a particular atom. This is achieved by starting at the given atom, visiting its neighboring atoms recursively, and marking each visited atom to prevent revisiting. Once all connected atoms have been found, they are returned as a list. The implementation of the DFS algorithm in the plugin is recursive, meaning that each function call results in another function call until the base case is reached.

Analyses

This customized Molecular Network plug-in for Nanome provides a powerful tool for the analysis and manipulation of molecular structures. The plug-in is designed to identify atoms in protein structures that have no direct connections to other atoms within the same residue or to atoms in neighboring residues. Such atoms are important because they may be more exposed to solvent and could play a role in ligand binding or protein-protein interactions. The plugin takes a protein structure in PDB format as input and identifies atoms that have no direct connections using network analysis algorithms. The output is a list of atoms with their corresponding residue and chain IDs. The plugin could be useful for protein structure analysis and drug design studies, as identifying these unconnected atoms could reveal potential binding sites or help explain protein function. Another important application of this plug-in is in the field of materials science. By analyzing the connectivity between atoms in a material, researchers can gain insight into its properties and behavior. This is critical for the development of new materials with specific properties, such as high strength or conductivity.

Results

```
Atom name:  O  , Location: (117.494, 83.999, 119.739)
Atom name:  CB , Location: (115.432, 83.954, 122.758)
Atom name:  CG , Location: (116.353, 84.424, 123.858)
Atom name:  CD , Location: (115.826, 84.073, 125.23)
Atom name:  OE1, Location: (114.772, 83.455, 125.359)
Atom name:  NE2, Location: (116.553, 84.472, 126.265)
Enter the x, y, and z coordinates of an atom(DO NOT include brackets): 116.353, 84.424, 123.858
Enter a distance parameter in Angstrom: 3
Atom name:  CA , Location: (115.803, 84.468, 121.372), Distance: 2.5464940604682385
Atom name:  CB , Location: (115.432, 83.954, 122.758), Distance: 1.5096824169341103
Atom name:  CG , Location: (116.353, 84.424, 123.858), Distance: 0.0
Atom name:  CD , Location: (115.826, 84.073, 125.23), Distance: 1.5110638636404519
Atom name:  OE1, Location: (114.772, 83.455, 125.359), Distance: 2.3856913044230916
Atom name:  NE2, Location: (116.553, 84.472, 126.265), Distance: 2.415771719347667
There are  6  atoms within the desired parameter
Atoms directly connected to the atoms within the desired parameter:
Atom name:  C  , Location: (114.113, 85.122, 119.77)
Atom name:  O  , Location: (114.353, 86.32, 119.943)
Atom name:  N  , Location: (114.748, 84.164, 120.429)
Atom name:  C  , Location: (117.12, 83.862, 120.903)
Atom name:  O  , Location: (117.494, 83.999, 119.739)
Atom name:  CB , Location: (115.432, 83.954, 122.758)
Atom name:  CG , Location: (116.353, 84.424, 123.858)
Atom name:  N  , Location: (114.748, 84.164, 120.429)
Atom name:  CA , Location: (115.803, 84.468, 121.372)
Atom name:  C  , Location: (117.12, 83.862, 120.903)
Atom name:  CG , Location: (116.353, 84.424, 123.858)
Atom name:  CD , Location: (115.826, 84.073, 125.23)
Atom name:  OE1, Location: (114.772, 83.455, 125.359)
Atom name:  CA , Location: (115.803, 84.468, 121.372)
Atom name:  C  , Location: (117.12, 83.862, 120.903)
Atom name:  CB , Location: (115.432, 83.954, 122.758)
Atom name:  CD , Location: (115.826, 84.073, 125.23)
Atom name:  OE1, Location: (114.772, 83.455, 125.359)
Atom name:  NE2, Location: (116.553, 84.472, 126.265)
Atom name:  OD2, Location: (113.402, 86.039, 125.282)
Atom name:  CB , Location: (115.432, 83.954, 122.758)
Atom name:  CG , Location: (116.353, 84.424, 123.858)
Atom name:  OE1, Location: (114.772, 83.455, 125.359)
Atom name:  NE2, Location: (116.553, 84.472, 126.265)
Atom name:  OD2, Location: (113.402, 86.039, 125.282)
Atom name:  CB , Location: (115.432, 83.954, 122.758)
Atom name:  CG , Location: (116.353, 84.424, 123.858)
Atom name:  CD , Location: (115.826, 84.073, 125.23)
Atom name:  NE2, Location: (116.553, 84.472, 126.265)
Atom name:  CG , Location: (116.353, 84.424, 123.858)
Atom name:  CD , Location: (115.826, 84.073, 125.23)
Atom name:  OE1, Location: (114.772, 83.455, 125.359)
main took 12.411549 ms to run
```



Conclusions

The Nanome Molecular Visualization platform offers precise visualization and analysis for complex molecular structures. The Molecular Network plug-in we developed, in particular, offers a user-friendly interface for exploring the connectivity of atoms within a molecule. This plugin has the potential to significantly enhance the efficiency and accuracy of research in various fields such as drug discovery, materials science, and biochemistry. With the ability to analyze molecular networks and identify key structural features, researchers can gain insights that would have been difficult or impossible to obtain with traditional methods. The user simply inputs the data by importing the molecular structure file into the Nanome software. And the plugin then processes the data by parsing the structure file and identifying the connectivity between the atoms. The outputs will present a list of all the atoms in the molecule, with their respective atomic symbols, names, and whether or not they are directly connected to another atom. The plugin also provides the option to output the list to a CSV file for further analysis. In short, the Nanome platform and Molecular Network plugin provide a valuable resource for researchers at all levels, from students to professionals. The platform's intuitive interface and powerful capabilities make it an excellent tool for exploring and understanding molecular structures, and we believe it will continue to play an increasingly important role in scientific research.

References

Plugin API — Nanome-Plugin-API documentation. (2023). Readthedocs.io. https://nanome.readthedocs.io/en/latest/plugins.html

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