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VEGA: a versatile program to convert, handle and visualize molecular structure on Windows-based PCs

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Abstract

We here propose the program VEGA, that was developed to create a bridge between the most popular molecular software packages. In this tool some features are implemented some features to analyze, display and manage the three dimensional (3D) structure of the molecules. The most important features are (1) file format conversion (with assignment of the atom types and atomic charges), (2) surface calculation and (3) trajectory analysis. The executable and the source code can be free downloaded from http://users.unimi.it/~ddl. © 2002 Elsevier Science Inc. All rights reserved.

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1. Introduction

The two quests, that VEGA can satisfy, can be reassumed into:

- The need of a program able to convert the file formats (assigning the atomic charge and the atom types) in order to help the data interchange.
- The need of a molecular visualization software for Windows-based PCs not only able to read (and save in) several file formats, but also capable to compute molecular surfaces and to analyze molecular trajectories. During the trajectory analysis, VEGA can calculate for each frame several molecular properties in order to gain a dynamic profile of their behavior in the time.

There are some programs that perform one of these functions (like Babel [1] for conversion of files or RasMol [2], VMD [3], Qmol [4], etc. for molecular visualization), but there are no software (especially for PCs), that share both functions.

2. Features

2.1. Input/output operations

- The supported file formats are: MSI Quanta/CHARMm CRD, Cambridge Data File (CSSR), Gromos, interchange file format (IFF), Tripos Sybyl (Mol2), HyperChem (.hin), MSI Quanta MSF, protein data bank ((PDB) and PDB not standard), protein data bank fat (PDBF), MSI/Biosym Insight II (.car), MOPAC internal co-ordinates, Cartesian co-ordinates (XYZ).
- An intelligent algorithm implemented in VEGA recognizes automatically the input file format.
- It is possible to load more than one file at once with the same or different file formats to create a molecular assembly. The calculation of connectivity is performed separately for each loaded file to prevent the connectivity errors of bumping molecules.
- The Data De/compressor Engine allows the use of the compressed files without previous un/packing operations: packed files can be managed in the same way of the unpacked files without any external data de/composer. VEGA supports the following packing formats: BZip (.bz2), GZip (.gz), PowerPacker (.pp) and Unix compress (.Z).
- Assignment atomic charge and atom typing (using a specified force field template).

2.2. Three dimensional graphic features

- Strong OpenGL [5] hardware acceleration (depending on the graphic card) with three dimensional (3D) object manipulation, interactively selection of atoms, lighting and smooth animations.
- 3D molecule view (wireframe, CPK wireframe, CPK solid, van der Waals wireframe, van der Waals dotted,

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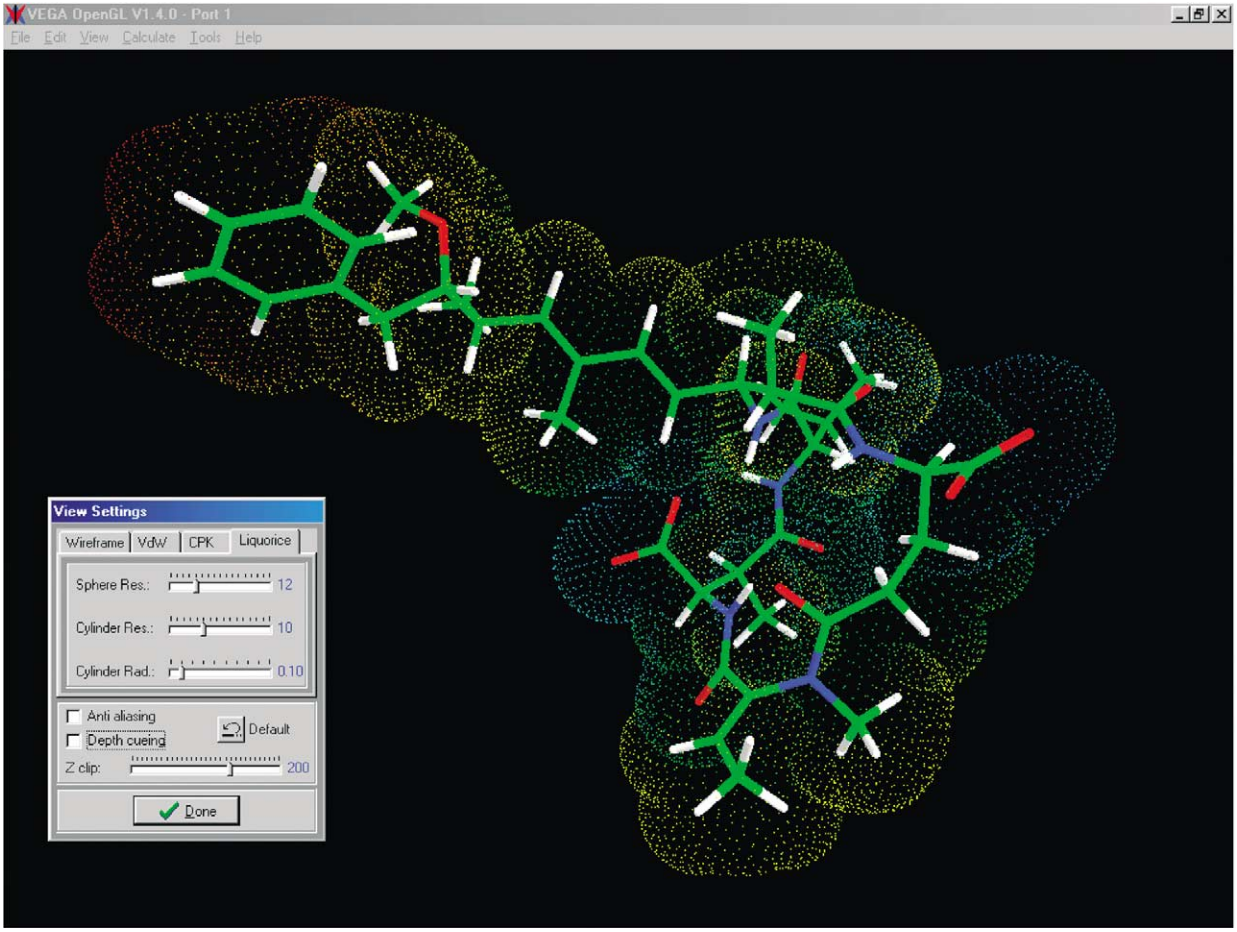

Fig. 1. Cyanobacterial toxin (PDB entry code 1EVD) in liquorice display mode (see the view settings for the liquorice properties) with MEP surface.

van der Waals solid and liquorice) with depth-cueing and anti-aliased lines.
- Molecule coloring (by molecule, by residue, by atom, by charge).

2.3. Surface features

- VEGA can calculate and display several types of molecular surface. The surfaces can be colored by specified color, by atom and by property (Fig. 1). It is possible to analyze some local molecular properties like hydropathicity (ILM hydropathicity surface [6] and polar surface area (PSA)), lypophilicity (molecular lipophilic potential (MLP) [7]), and molecular charges (molecular electrostatic potential (MEP)).
- VEGA can read and save the surface files, supporting the Biosym surface format (formatted file) and the Quanta surface format (binary file).
- Vega can use also the virtual reality modeling language (VRML) [8] in order to support the web publishing. The surface can be stored in VRML as dotted or solid surface.

2.4. Trajectory analysis

- VEGA can analyze the trajectory file of a molecular dynamic simulation, displaying the results with a 2D/3D/4D graphical representation and with the animation of molecular trajectory (Fig. 2).
- At the present time, only the CHARMm/XPLOR format (.DCD [9]) is implemented. To read DCD files created with a variety of computer architectures, VEGA recognizes automatically both big- and little-endian data formats.
- The molecular properties, that VEGA can calculate for each frame of the trajectory, are bond angle, bond length, torsion angle, angle between planes, molecular dipolar moment, surface area, molecular volume, virtual $\log P$ and polar surface area.
- The results can be highlighted using a Graph Editor that allows to show and to manage data sets calculated by VEGA and/or by other external programs. This Graph Editor has the following functions:
  - The supported file formats are: CHARMM .ene, comma separated values .csv, Quanta .plt and Custom.

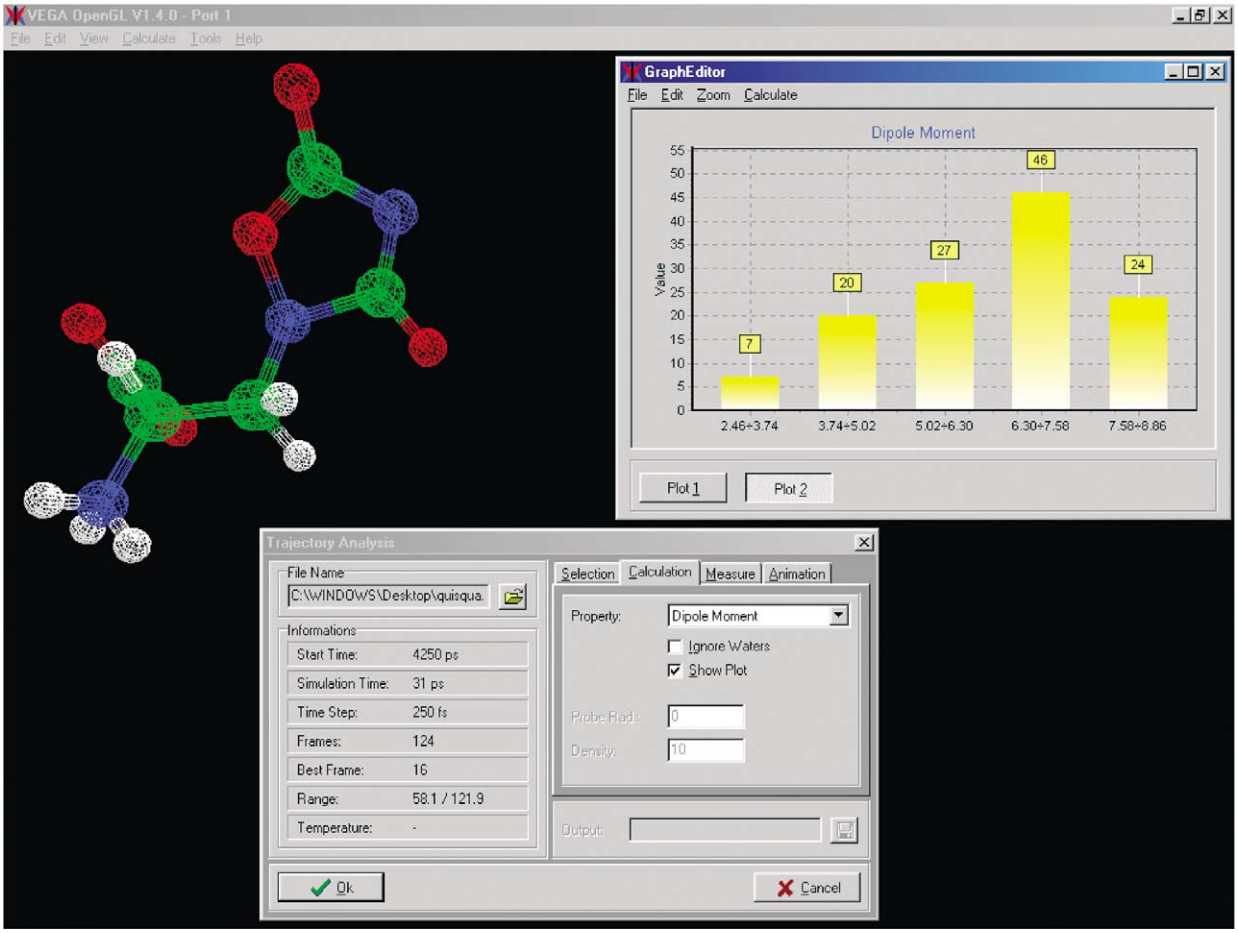

Fig. 2. Display of the results of an MD trajectory of the quisqualic acid. In the figure you can note the trajectory analysis dialog box and the cluster analysis of the dipole values.

An autodetect routine recognizes the correct file format, during the loading operations. However, if the data set format is ASCII, you can use a suitable filter in order to select the data (X and Y columns).

- Zoom function to select a specific plot area.
- Clustering function in which it is possible to define the number or the ranges of the clusters. The clustering analysis produces an histogram in which are represented the number of values contained in each cluster.

3. Conclusion

Even if without graphical interfaces, VEGA runs also on other operating systems, like UNIX, Linux, IRIX, and AmigaOS. In these environments VEGA uses a command line interface and it performs all the functions examined in Windows version (file conversion, surface calculations, trajectory analysis and structure handling).

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