Journal of Cheminformatics

ORAL PRESENTATION Open Access

CELLmicrocosmos 2.2: advancements and applications in modeling of three-dimensional PDB membranes

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From 5th German Conference on Cheminformatics: 23. CIC-Workshop
Goslar, Germany. 8-10 November 2009

Background

Today, only a few programs support membrane computation and/or modeling in 3D. They enable the user to create very simple-structured membrane layers and usually assume a high level of bio-chemical/-physical knowledge. The CELLmicrocosmos 2 project developed a tool providing a simplified workflow to create membrane (bi-)layers: The MembraneEditor (CmME).

Results

The geometry-based, scalable and modular computation concept supports fast to more complex membrane generations. CmME is based on the integration of two different types of PDB [1] models: Lipids are integrated with editable percental distribution values and algorithms. Proteins are inserted and aligned into the bilayer manually or automatically, by using data from the PDB_TM [2] or OPM [3] database. Compatibility with other programs is offered by extensive PDB format export settings. High lipid densities are possible through advanced packing algorithms. Lipid distributions can be developed by using the Plugin-Interface. Originally not intended to change the atomic structure of the molecules due performance issues, now it is also possible to access the atomic level for user-defined computations. Multiple membrane (bi-)layers and microdomains are supported as well as a reengineering function providing the re-editing of externally simulated PDB membranes.

Conclusions

The capabilities of CmME has been extended and tested to meet the requirements of different PDB visualization programs as well as molecular dynamics (MD) simulation environments like Gromacs [4]. The documentation and the Java Webstart application, requiring only an internet connection and Java 6, is accessible at: http://Cm2.CELLmicrocosmos.org

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Published: 4 May 2010

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doi:10.1186/1758-2946-2-S1-O21
Cite this article as: Sommer *et al.*: CELLmicrocosmos 2.2: advancements and applications in modeling of three-dimensional PDB membranes. *Journal of Cheminformatics* 2010 **2**(Suppl 1):O21.

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