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CELLmicrocosmos 2.1: a software approach for the modelling of three-dimensional PDB membranes

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Background

CELLmicrocosmos is an approach to develop tools for the generation of virtual cell environments. The CELLmicrocosmos 2 project deals with the computational generation of three-dimensional cell membranes. Biological membranes consist mainly of lipids and proteins. The Protein Data Bank [1] and the HIC-UP database [2] represent a large number of three-dimensional protein and lipid structures, which have been extracted from biological membranes. Other databases contain information about the membrane-type-specific localization of proteins. There exist various approaches of utilizing these models for the computation of membranes.

Results

Research in many fields of science is dealing with the problem of visualizing, modelling and/or simulating membranes. The theoretical as well as the computational status quo does not allow to generate realistic membranes. Hence, alternatives are created, which are using different developmental environments. Therefore a lot of work has to be invested, before the sophisticated work dealing with algorithms can begin.

We present a software framework, which should allow academics to generate problem-specific membranes: They should be enabled to use simple, short-time as well as complex, time-consuming algorithms featuring a higher grade of realism.

Conclusion

Utilizing Java, Java3D and Jmol [3], we created a tool which is able to deal with different PDB models. While proteins are aligned manually, a number of algorithms for the percental lipid distribution has been implemented. The most sophisticated one so far is a geometrical-based Monte Carlo algorithm. The exported PDB membranes could be used to run Molecular Dynamics simulations with appropriate programs.

References

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