

Poster presentation

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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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