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

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## 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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## References

1. Berman HM, Westbrook J, Feng Z, Gilliland G, Bhat TN, Weissig H, Shindyalov IN, Bourne PE: **The Protein Data Bank**. *Nucleic Acids Research* Oxford University Press, Oxford 2000, **28**:235-242.
2. Tusnady GE, Dosztanyi Z, Simon I: **Transmembrane proteins in the Protein Data Bank: identification and classification**. *Bioinformatics* 2004, **20**(17):2964-2972.
3. Lomize MA, Lomize AL, Pogozheva ID, Mosberg HI: **OPM: Orientations of Proteins in Membranes database**. *Bioinformatics* 2006, **22**:623-625.
4. Lindahl E, Hess B, Spoel van der D: **GROMACS 3.0: A package for molecular simulation and trajectory analysis**. *J Mol Mod* 2001, **7**:306-317.

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