Open Babel

Open Babel is computer software, a chemical expert system mainly used to interconvert chemical file formats.[2] Due to the strong relationship to informatics this program belongs more to the category cheminformatics than to molecular modelling. It is available for Windows, Unix, Linux, macOS, and Android. It is free and open-source software released under a GNU General Public License (GPL) 2.0.

The project's stated goal is: "Open Babel is a community-driven scientific project assisting both users and developers as a cross-platform program and library designed to support molecular modeling, chemistry, and many related areas, including interconversion of file formats and data."

Contents

- History
- Major features
- See also
- References
- External links

History

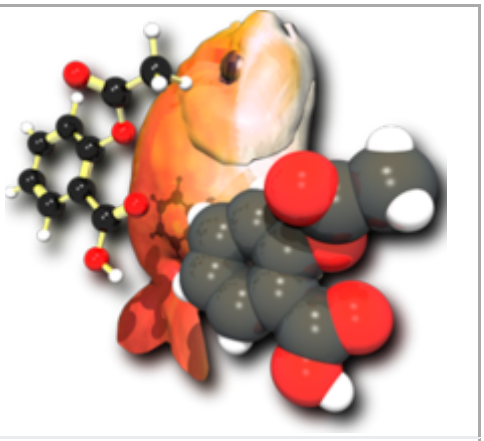
Open Babel and JOELib were derived from the OELib cheminformatics library. In turn, OELib was based on ideas in the original chemistry program Babel and an unreleased object-oriented programming library called *OBabel*.

Major features

- chemical expert system
- interconversion of many chemical file formats
- substructure search, based on simplified molecular-input line-entry system (SMILES)
- fingerprint calculation
- 3D coordinate generation[3]
- wrappers for Python, Perl, Java, Ruby, C#[4]

See also

Open Babel



Developer(s)	Open Babel development team
Initial release	2 June 2005
Stable release	2.4.0 / 25 September 2016
Repository	github.com/openbabel/openbabel (https://github.com/openbabel/openbabel)
Written in	C++ (wxWidgets[1])
Operating system	Windows, macOS, Linux, Android
Platform	IA-32, x86-64
Available in	English
Type	Cheminformatics, molecular modelling
License	GPL 2.0
Website	openbabel.org (http://openbabel.org)

- Avogadro – molecular builder and editor based on Open Babel
- Ghemical – molecular mechanics program based on Open Babel
- JOELib – Java version of Open Babel and OELib
- XDrawChem – 2D drawing program based on Open Babel
- Comparison of software for molecular mechanics modeling
- Blue Obelisk[5]
- List of free and open-source software packages

References

1. "Debian -- Details of package openbabel-gui in jessie" (https://packages.debian.org/jessie/openbabel-gui). Retrieved 2017-03-10.
2. O'Boyle, N. M.; Banck, M.; James, C. A.; Morley, C.; Vandermeersch, T.; Hutchison, G. R. (2011). "Open Babel: An open chemical toolbox" (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3198950). *Journal of Cheminformatics*. **3**: 33. doi:10.1186/1758-2946-3-33 (https://doi.org/10.1186%2F1758-2946-3-33). PMC 3198950 (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3198950). PMID 21982300 (https://pubmed.ncbi.nlm.nih.gov/21982300).
3. Yoshikawa, Naruki; Hutchison, Geoffrey R. (1 August 2019). "Fast, efficient fragment-based coordinate generation for Open Babel" (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6676618). *Journal of Cheminformatics*. **11** (1): 49. doi:10.1186/s13321-019-0372-5 (https://doi.org/10.1186%2Fs13321-019-0372-5). PMC 6676618 (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6676618). PMID 31372768 (https://pubmed.ncbi.nlm.nih.gov/31372768).
4. http://openbabel.org/
5. Guha, R.; Howard, M. T.; Hutchison, G. R.; Murray-Rust, P.; Rzepa, H.; Steinbeck, C.; Wegner, J.; Willighagen, E. L. (2006). "The Blue Obelisk - Interoperability in Chemical Informatics" (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4878861). *Journal of Chemical Information and Modeling*. **46** (3): 991–998. doi:10.1021/ci050400b (https://doi.org/10.1021%2Fci050400b). PMC 4878861 (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4878861). PMID 16711717 (https://pubmed.ncbi.nlm.nih.gov/16711717).

External links

- Official website (http://openbabel.org)
- E-BABEL (http://www.vcclab.org/lab/babel) – interactive version of the Open Babel at Virtual Computational Chemistry Laboratory
- chemCast Episode 003 (https://web.archive.org/web/20070928203357/http://chemcast.org/podcast/?p=7) – project lead developer Geoff Hutchison was interviewed on the podcast
- Design flaws in OELib (https://web.archive.org/web/20070623080733/http://www.eyesopen.com/products/toolkits/OEChem/decision.html)