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Dingo: 2D molecule and reaction structural formula rendering library

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2D structural formulae are widely accepted as a way of representing chemical compounds and reactions. High-quality visualization of those formulae can greatly facilitate scientist perception.

We are proud to present a tool for such visualization, called Dingo [1]. It is capable of rendering molecules, reactions and queries along with a wide range of attributes on Windows, Linux, Solaris and Mac OS in accordance with IUPAC recommendations [2].

Dingo accepts common file formats, such as MDL Molfile [3] and Rxnfile, SMILES [4] with several extensions and more. The result can be stored as a PDF, SVG, PNG or EMF file. One can also embed Dingo in an application and use it via simple C interface or a C# wrapper to produce image files or render directly to a Windows HDC.

Dingo is a strong competitor for existing proprietary tools on the market, while it is available under the terms of GPLv3 free of charge.

The aim of the project is to provide a simple and efficient mechanism for 2D structural formula rendering. High quality and the variety of supported formats allows inclusion of resulting images in scientific papers, further editing of the output in a vector form or embedding the library in more complex applications.

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References

1. [<http://opensource.scitouch.net/indigo/dingo>].
2. [<http://www.iupac.org/objID/Article/pac8002x0277>].
3. [<http://www.symyx.com/downloads/public/ctfile/ctfile.pdf>].
4. [<http://www.daylight.com/smiles/>].

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