

# LEXICHEM

Accurate modeling requires 3D structures, so a lot of attention is paid to them. However, chemists often do not think in 3D, identifying compounds instead by name or 2D Kekule drawing. LexiChem and Ogham provide the chemical language more familiar to that audience. LexiChem provides efficient conversion of chemical names to chemical structures and *vice versa*, where chemical names can be standard IUPAC names or more common traditional names, while LexiChem's companion product, Ogham, provides useful 2D renderings.

LexiChem's speed and high conversion rate makes it an attractive tool for a number of uses. The San Francisco-based software firm, Reel Two, uses it in SureChem, a program for extracting compound information from literature and patents. According to Reel Two's Senior Vice-President, Nicko Goncharoff, "LexiChem allows us to easily offer methods of chemical compound searching that would be difficult to achieve otherwise."

The primary features of LexiChem include:

- Gives reasonable names to chemical structures or connection tables
- Generates accurate connection tables for named compounds
- Understands and writes several naming styles including fully systematic, preferred IUPAC 2005, acceptable common-usage IUPAC, CAS, and traditional
- OEChemplete – all I/O and molecular information processing by OEChem
- OEChempatible C++ toolkit for embedded applications
- Robust reading and specification-compliant writing of SMILES, SLN, SDF, MOL, MOL2, PDB, FASTA, MOPAC, MacroModel, XYZ, and OEBinary file formats
- Support for LINUX, IRIX, Windows, OS X, AIX, HP-UX, Solaris, Tru64UNIX



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