

Supporting technologies

Ceres [↗](#)

A Lhasa built java chemical engine library used in various cheminformatics applications. It is part of a suite of tools that provide functionalities for handling molecular structures and transformations. There are two flavors MoonCeres, maintained by the MIT team and SD Ceres used primarily in member facing solutions.

Amongst other functions, It can be used to convert molecular structures expressed in one format, into another. As Vitic expects molecular structures in Mol format, we may consider including this in the POC system.

OPSIN: Open Parser for Systematic IUPAC Nomenclature

Open Parser for Systematic IUPAC Nomenclature (OPSIN). It's a free, open-source software tool used for converting chemical names into chemical structures. Developed by the University of Cambridge, it's particularly useful for researchers, chemists, and software developers working with chemical informatics.

OPSIN can interpret and parse systematic IUPAC (International Union of Pure and Applied Chemistry) names and generate corresponding molecular structures, typically in formats like SMILES, InChI, or MOL. This is helpful in cheminformatics applications where understanding or visualizing a chemical from its name is necessary.

If you're dealing with chemical data, OPSIN can be integrated into other software or used through its web interface for quick conversions.