

SMACK

SMACK [1] converts and optimizes molecular database queries. SMACK can quickly convert from substructure and reaction queries expressed in MDL file format to SMARTS strings. Additionally, SMACK will automatically optimize each resulting query for pattern-matching performance. Typical transformations simplify redundant atom and bond expressions and reorder atoms for faster matching against medicinal/organic chemistry databases.[2] SMACK will, of course optimize a SMARTS query for output in the same format.

"SMACK is an important component of Vertex's Cheminformatics infrastructure," stated Patrick Walters, Ph.D., Principal Investigator, of Vertex Pharmaceuticals. "SMACK has been used to convert tens of thousands of queries over the past three years. We have been consistently impressed by the program's performance and the support provided by the OpenEye staff".

The primary features of SMACK include:

- Reads queries in MDL file formats – Mol, RG, Rxn – from programs such as MDL's ISIS/Draw or CambridgeSoft's ChemDraw [3]
- Reads and writes SMARTS and SMIRKS queries for instance for Daylight's DayCart or Merlin database systems [4]
- Converts queries from MDL to SMARTS
- Optimizes queries for database searching [2]
- Support for LINUX, HP-UX, Tru64UNIX, AIX, IRIX, Solaris, Windows, OS X
- Available on request as a C++ toolkit for embedded applications.



[1] Because after something is SMACKed, it SMARTS.

[2] 1st-Class SMARTS Patterns: Sayle, R., Daylight *EuroMUG 97*, Verona, Italy, October 1997, <http://www.daylight.com/meetings/emug97/Sayle/>

[3] MDL CTFfile formats: <http://www.mdli.com/downloads/public/ctfile/ctfile.jsp>

[4] Daylight SMARTS and SMIRKS: <http://www.daylight.com/dayhtml/doc/theory/theory.smarts.html>

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