Daylight

Chemical
Information
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What's new in version 4.83

Euromug 2004

Documentation references

http://www.daylight.com/dayhtml/doc/release_notes/readme_v483.html

Overview

- Version 4.83 is a cumulative patch, so it includes all of the changes which were introduced in the 4.82 patch.

- The 4.82 changes included bug fixes, new Daycart features, new HTTP toolkit-based SMI2GIF and DEPICT utilities, and the new property package.

- New features specific to Version 4.83 include bug fixes, new DayPerl, new Daycart Optimizer code, additional Depiction control over layout, and a first public Windows toolkit/Daycart release (beta).

Documentation

- As with all releases, documentation of the changes is in text files in $DY_ROOT.
  - readme-v*nnn*
  - readme-v*nnn-operating_system*
- In addition the same material is available at
  http://www.daylight.com/dayhtml/doc/release_notes/readme_v*nnn*.html
- For convenience a local copy is available here

New DayPerl

- A completely new build procedure for DayPerl eliminates many of the version related problems with the previous build. The new build files are in $DY_ROOT/contrib/src/perl/DAYPERL_BUILD/

- Compiled Dayperl files can be downloaded from
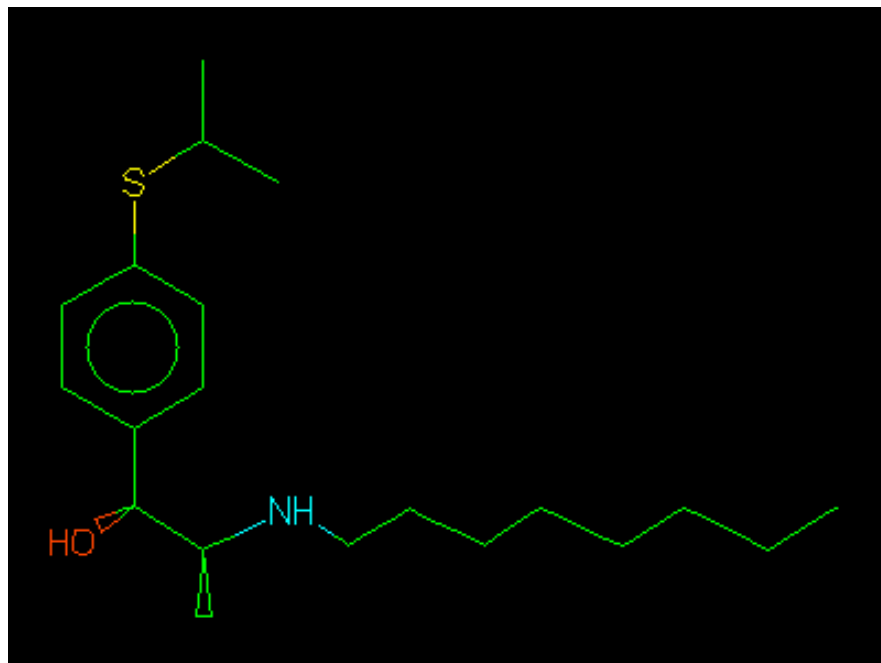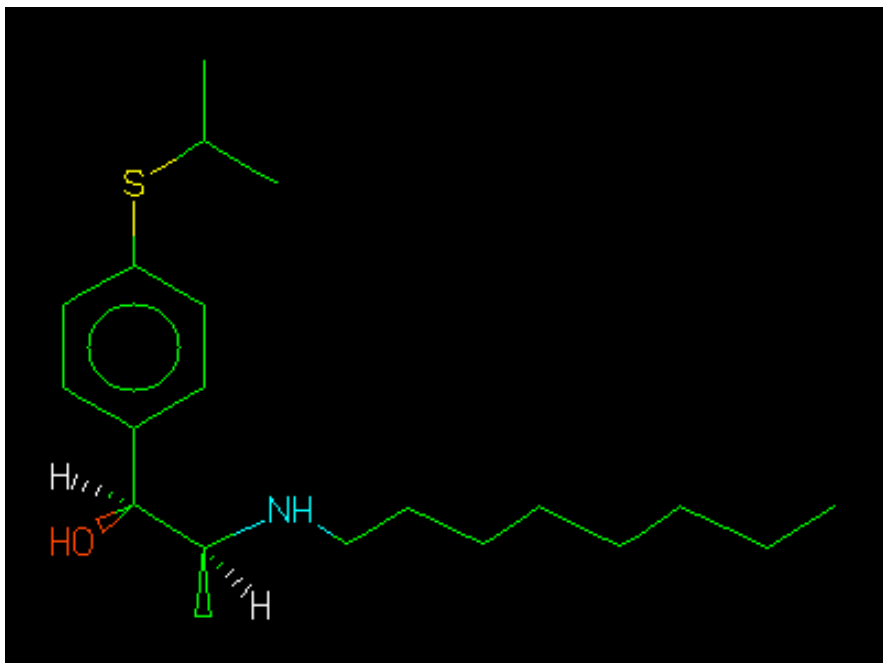 http://www.daylight.com/support/contrib/dayperl

New Daycart Optimizer Code

- A new, *experimental* optimizer package is included with Daycart in this version. It is specific to Oracle 9i and 9iR2 and gives the user the ability to query and scale the statistics provided to Oracle. See the file $DY_ROOT/dcischem/README.optimizer9 for details.

- Note in particular we ask you DO NOT use this package on a production Oracle database!!! Only after thorough testing and positive customer feedback will this optimizer package be included in a release (probably 4.91) in supported form.

- Take the opportunity to talk with Jack and Kathy about this during the meeting.

Depiction Options

- Depiction objects now pay attention to three new named properties: "old_style", "hide_chi_h", and "hlen_pct". These are documented in $DY_ROOT/man/man3ob/depiction.3ob. Also at http://www.daylight.com/dayhtml/doc/man/man3ob/depiction.html . For convenience the current copy is here.

- Programs which use depictions obey the options:
  - DEPICT_OLD_STYLE
  - DEPICT_HIDE_CHI_H
  - DEPICT_HLEN_PCT

- These control these three style options globally in each program.

- They are regular options so can be set site-wide, for an individual user or for a particular run with a particular program.
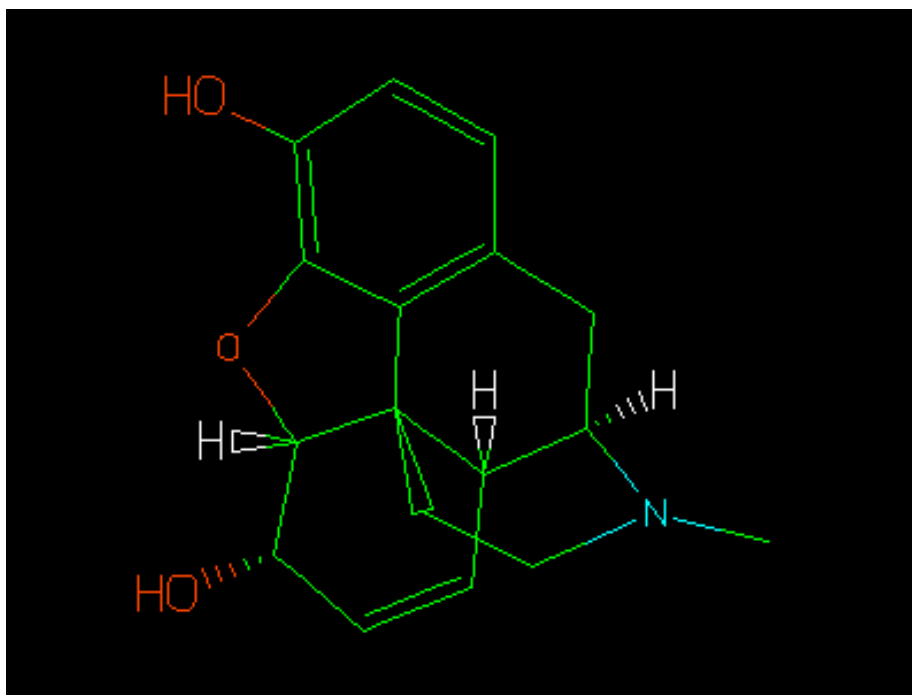
Hide chiral H's

Effect of setting DEPICT_HIDE_CHI_H to be TRUE

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Web based depiction

- URL's pointing to a dayhttp server understand these new options in the form
  - http://www.daylight.com/dayhttp/smi2gif?hide_chi_h=true&hlen_pct=0.75&xsmiles=true
- <u>Other than xsmiles none of these options are available in the daycgi version</u>
- For example
  - http://www.daylight.com/dayhttp/smi2gif?hide_chi_h=true&hlen_pct=0.75&xsmiles=true&tdt=%24SMI%3CCN1CC%5BC%40%5D23%5BC%40H%5D4Oc5c3c(C%5BC%40%40H%5D1%5BC%40%40H%5D2C%3DC%5BC%40%40H%5D4O)ccc5O%3E2D%3C2.76%2C-1.20%2C1.87%2C-0.98%2C0.89%2C-1.40%2C0.02%2C-0.97%2C-0.20%2C-0.15%2C-0.98%2C-0.42%2C-1.52%2C0.34%2C-0.92%2C1.03%2C-0.16%2C0.66%2C0.60%2C1.09%2C1.38%2C0.61%2C1.32%2C-0.31%2C0.51%2C-0.68%2C0.41%2C-1.57%2C-0.45%2C-1.91%2C-1.16%2C-1.31%2C-2.01%2C-1.61%2C0.60%2C2.01%2C-0.21%2C2.46%2C-0.99%2C1.96%2C-1.79%2C2.35%3B%3E%7C

Web Example

Morphine depicted using coordinates from wdi and options
"hide_chi_h=true&hlen_pct=0.75&xsmiles=true&"

Windows Toolkits and Daycart

- The Toolkits and Daycart are available under Windows in native form. This is a public beta release.

- This is the subject of a separate talk.

- But….

Bug fixes

- ## Depictions
  - Tetrahedral chiral centres with double bonds (eg. [P]) were not depicted correctly; the double bond was drawn as single. The current fix is for bond-order to take priority over bond-style. This is like ISIS-Draw behaviour for chiral S-oxides etc.
  - EZ depictions were often laid out incorrectly. The tee indicators are always correct, now the actual layout actually matches the tee indicators.
  - Note neither of these affect the underlying structure which was *always* held correctly

- ## Linking
  - __ctype_b, __ctype_tolower, __ctype_toupper are unresolved symbols on RH9, RHES3. These were eliminated from GLIBC in favor of localization-aware versions.

Thor

- Thor graph normalization incorrectly rejected structures with isolated hydrogens.

- Previously, when creating thor databases, the hashtable cache value was set to "ALWAYS" by default; it was possible to create a database that could not be opened (if the cached hashtable was larger than the memory available). The new default is "ON REQUEST". To get the old behavior, use "-CACHE_WHEN ALWAYS" with thormake.

- In thorload, the error queue wasn't cleared until messages are printed; irrelevant messages would accumulate and eventually get dumped out.

Merlin

- MCL no longer printed the hitlist position or length.

- Print hitlist from xvmerlin (using tablet) would not depict structures unless the columns were named SMILES, Isomer, or IsomSMILES. Now obeys the option -PRINT_DEPICT which lists the structural column names.

- Recursive SMIRKS with dot-separated recursive expressions were incorrectly parsed.

- The file widget dropped entries if the directory contained more than 1000 entries.

DayCart

- The vcs_normalize() function in Daycart always returned the isomeric SMILES; it ignored the 'iso' parameter

Reminder

- Complete documentation of the changes and bug fixes is in text files in $DY_ROOT.
  - readme-v4*83*
  - readme-v*483-operating_system*

- In addition the same material is available at
  http://www.daylight.com/dayhtml/doc/release_notes/readme_v483.html

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