Daylight v4.91 Release

27 April 2005

Daylight
Chemical
Information
Systems, Inc.

Enterprise-level cheminformatics.

Daylight 4.91

PLATFORMS SUPPORTED	Toolkits	Applications	Servers	Daycart
Solaris - 7, 8, 9; both 32- and 64-bit	X	X	X	X
SGI - Irix 6.5; both 32- and 64-bit	X	X	X	
IA32 - RH ES2.1, ES3,ES4	X	X	X	X
Mac - 10.3 (32-bit)	X	X	X (no Xwin)	
MSWindows - 2000 Professional, XP, 2003 Server	X			X
Oracle - 9iR2, 10g				X
NEW				
AMD64 - RH ES3, Suse8.	X	X(32-bit)	X	X
Solaris 10	X	X	X	X
Fedora	X	X	X	X

REMOVING
Irix 6.4
RedHat 7.1-9
Oracle 8i, 9.0x

4.91 DayCart Additions

- Oracle 10g (Never Breaks™)
  - Supported across our Solaris, IA32, AMD64, and MS platforms
  - Better integration of CLOBs
  - More parallelization
- Internationalization
  - Support for 120/257 Oracle character sets
  - Supersets of ASCII
  - most European sets and major Unicode versions

4.91 DayCart Additions

- Partitioned tables and indexes
    - Oracle 9i and 10g
    - Range partitioned on one column
    - Improved search speed
- More flexible similarity searches
    - ... tanimoto(smi, 'c1ccccc1') > 0.9
    - ... similarity(smi, 'c1ccccc1', 'TANIMOTO') > 0.9
    - ... similarity(smi, 'c1ccccc1', 'c/(a+b+c)') > 0.9
- Reaction enumeration in Oracle 9iR2 and 10g
    - Ability to generate combinatorial libraries

4.91 DayCart Additions

- Optimizer Package
  - Functions to get functional CPU cost, IO cost, and selectivity for a query (contains, matches, exact)
  - Functions to get index path CPU cost and IO cost
  - Function parameters for ddpackage finfo() and fsetinfo() to manage scaling factors
    - Separate control of function and index execution paths
    - Parameters can be changed between SQL queries but not within a query

4.91 DayCart Additions

- Smi2pmw - precise molecular weights (IUPAC 2001)
- Error queue information exposed
- Memory usage issues resolved
- ddpackage specification unwrapped

4.91 Feature/Product Additions

- New Product - Conversion Package (molecules)
  - Command line and DayCart
- Feature Additions - Depiction TK
  - Improved control of layout, hydrogens & stereo display
  - Improvements to smi2gif
- Feature Additions - Clustering Package
  - Spherex - Sphere exclusion
  - Kmodes - Kmodes
  - Near neighbors - tie handling for JP
  - User-defined similarity expressions

4.91 Feature/Product Additions

- ## Feature Addition - Fingerprint TK
  - dt_fp_similarity(3) / expression(5)

- ## Feature Addition - Smiles TK
  - dt_smilin_addh(3) / dt_addh(3) / dt_suppressh(3)
  - dt_molgraph(3)
  - Bug fix - Directional (EZ) aromatic bonds in SMILES.

- ## Feature Addition - Properties Package
  - Tautomer enumeration

4.91 Feature/Product Additions

- Thor/Merlin
  - Thor: Large files under Linux.
  - Merlinserver: generic fingerprint search using dt_mer_similarselect(3)