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Daylight Print Manual

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PrintPackage Manual

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1. Intended audience and scope of this document.

This document should be read by everyone who intends to use the Daylight printing programs, collectively known as the Daylight "PrintPackage".

This Guide provides sufficient information for a novice Daylight user to successfully use the PrintPackage for a wide range of printing tasks. Additional relevant documentation can be found in the Daylight Theory Manual and Daylight Reference Manual (man pages) pertaining to the file formats used with the PrintPackage, such as TDT files, FDT files, and TAB files. The PrintPackage programs make use of the PostScript Level 2 printing language, by Adobe.

Also note that online help is available with each PrintPackage program by invoking the command-line option "-help".

2. Introduction to the Daylight PrintPackage

The Daylight PrintPackage is a set of programs which can convert data files written by Daylight programs such as THOR and Merlin to PostScript files. These files can include both text and structures extracted from a database, formatted in a variety of ways. It should also be noted that the PrintPackage programs are stand-alone programs and can process files not produced by Daylight software, for example, a tab-delimited spreadsheet dump.

The PrintPackage is responsible for producing PostScript files for printing or inclusion in another document. It is the responsibility of the local system manager to be able to print a PostScript file. However, some general guidelines are provided in Appendix 1 "Printing PostScript Files".

The PrintPackage currently is comprised of three programs: Treetops (for Thor data TREE TO PostScript), Prado (PRint A Depict Object), and Tablet. Treetops converts a 'Formatted Data Tree' file (FDT file) containing data for one or more substances to PostScript. FDT files are typically created by the Thor manager program Thorlookup (part of the ThorManager package). Prado writes a PostScript file of depictions for a list of input SMILES, in SMILES-file or TDT-file format. Tablet writes a table-style PostScript output file from an input TAB-file, which is typically written by Merlin for the current hitlist.

3. Treetops

Treetops is used for printing Thor data trees (TDTs). A good place to start learning Treetops usage is the online help text. We can produce this by entering "treetops -help" on the command line:

```
% treetops -help
treetops 4.71 Daylight CIS Inc. -- SYNTAX SUMMARY

Convert tab-delimited datatree to PostScript file with depictions

Usage:  treetops [options] < in.fdt > out.ps
or:    treetops [options] in.fdt > out.ps
or:    treetops [options] in.fdt out.ps

or:    treetops -help           (show this summary)
or:    treetops -notes         (show release notes)
or:    treetops -options       (show option summary)
or:    treetops -settings      (show current settings)
```

By entering "treetops -options" we can display a list of available options:

```
% treetops -options
treetops 4.71 Daylight CIS Inc. -- OPTION SUMMARY

Convert tab-delimited file to PostScript file with depictions

Usage:  treetops [options] < in.fdt > out.ps
or:    treetops [options] in.fdt > out.ps
or:    treetops [options] in.fdt out.ps

Page formatting options:
-DEPICT_SUPPRESS_LABELS  [TRUE|FALSE]
-PRINT_BINDER            [NONE|LEFT|TOP|LEFTRIGHT|TOPBOTTOM]
-PRINT_BOLDWIDTH        [THIN|NORMAL|WIDE|EXTRAWIDE]
-PRINT_COLORMODE        [BOW|WOB|COW|COB]
-PRINT_DATAFONT         "Helvetica"
-PRINT_DATASIZE         <size of font used for data, points>
-PRINT_FOOTER           NONE|STANDARD
-PRINT_LABELFONT        "Helvetica-BoldOblique"
-PRINT_LABELSIZE        <size of font used for labels, points>
-PRINT_LANGUAGE         PS|EPS
-PRINT_LINEWIDTH        [THIN|NORMAL|WIDE|EXTRAWIDE]
-PRINT_MARGINS          [BLEED|MINIMAL|NARROW|NORMAL|WIDE|HUGE]
-PRINT_ORIENT           [TALL|WIDE]
-PRINT_PAGELIMIT        <max number of pages to print>
-PRINT_PAPER            [USLETTER|USLEGAL|USTABLOID|A3|A4|A5|B5|
                        COMPUTER|FANFOLD]
-PRINT_PICTSIZE         <height of picture(s), points>
-PRINT_SMARTS           NONE or SMARTS to highlight
-PRINT_STEREO_ANG       <angular stereo separation, degrees>
-PRINT_STEREO_SEP       <stereo image pair separation, points>
-PRINT_TITLE            NONE or "any string"
-PRINT_TITLEFONT        "Helvetica-Bold"
-PRINT_TITLESIZE        <size of font used for title, points>

Data formatting options:
-PRINT_DEPICT           NONE or "tag,tag,...,tag"
-PRINT_SCHEMA           NONE or "tag,tag,...,tag"
-PRINT_STEREO           NONE or "tag,tag,...,tag"
```

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-PRINT_TEXT NONE or "tag,tag,...,tag"

By entering "treetops -settings" we can display the default values of all options:

```
% treetops -settings
treetops 4.72 (c) Daylight CIS Inc. -- CURRENT OPTION SETTINGS

DEPICT_SUPPRESS_LABELS .. TRUE
PRINT_BINDER ..... NONE
PRINT_BOLDWIDTH ... NORMAL
PRINT_COLORMODE ... BOW
PRINT_DATAFONT .... Helvetica
PRINT_DATASIZE .... 10.00
PRINT_DEPICT ..... SMILES|Isomer|Isomeric SMILES
PRINT_FOOTER ..... STANDARD
PRINT_LABELFONT ... Helvetica-BoldOblique
PRINT_LABELSIZE ... 10.00
PRINT_LANGUAGE .... PS
PRINT_LINEWIDTH ... THIN
PRINT_MARGINS ..... NORMAL
PRINT_ORIENT ..... TALL
PRINT_PAGELIMIT ... 100
PRINT_PAPER ..... USLETTER
PRINT_PICTSIZE .... 72.00
PRINT_SCHEMA ..... NONE
PRINT_SMARTS ..... NONE
PRINT_STEREO ..... 3D-coords|3D coords
PRINT_STEREO_ANG .. 5.00
PRINT_STEREO_SEP .. 196.00
PRINT_TEXT ..... NONE
PRINT_TITLE ..... NONE
PRINT_TITLEFONT ... Helvetica-Bold
PRINT_TITLESIZE ... 14.00
```

The Treetops options are described more fully below.

PAGE FORMATTING OPTIONS:

DEPICT_SUPPRESS_LABELS

Suppress atom labelling for chains, one of [TRUE | FALSE].

PRINT_BINDER

If the pages printed are to be bound, appropriate spacing can be specified. Select one of: [NONE | LEFT | TOP | LEFTRIGHT | TOPBOTTOM].

PRINT_BOLDWIDTH

Specify the width of the lines used for highlighted parts of depictions, one of [THIN | NORMAL | WIDE | EXRTAWIDE].

PRINT_COLORMODE

Specify black-on-white, white-on-black, color-on-white, or color-on-black, one of [BOW | WOB | COW | COB].

PRINT_DATAFONT

Font for character data.

PRINT_DATASIZE

Size of font used for character data, in points.

PRINT_FOOTER

Print footer information and page number; one of [STANDARD|NONE].

PRINT_LABELFONT

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- Font for datatypes, footers, etc.
- PRINT_LABELSIZE**
Size of font used for labels.
- PRINT_LANGUAGE**
Format of output file, one of [PS|EPS]. PS (PostScript) is used to print directly, EPS (Encapsulated PostScript) is often used to include graphics within another document.
- PRINT_LINEWIDTH**
Specify the width of the lines used for depictions, one of [THIN | NORMAL | WIDE | EXRTAWIDE].
- PRINT_MARGINS**
One of: [BLEED | MINIMAL | NARROW | NORMAL | WIDE | HUGE].
- PRINT_ORIENT**
One of [TALL | WIDE].
- PRINT_PAGELIMIT**
Maximum number of pages to print.
- PRINT_PAPER**
Paper size; choose one of [USLETTER | USLEGAL | USTABLOID | A3 | A4 | A5 | B5 | COMPUTER | FANFOLD].
- PRINT_PICTSIZE**
Size for structural depictions in points.
- PRINT_SMARTS**
Specifying a SMARTS with this option will highlight the atoms of the hit SMARTS in the input structures if there is a hit.
- PRINT_STEREO_ANG**
Stereo viewing angle for stereo depiction of conformations, in degrees.
- PRINT_STEREO_SEP**
Stereo image pair separation distance, in points.
- PRINT_TITLE**
Title for output document; appears at the top of each page.
- PRINT_TITLEFONT**
Font for title.
- PRINT_TITLESIZE**
Size of font used in title, in points.

DATA FORMATTING OPTIONS:

- PRINT_DEPICT**
Specify which datatypes are to be depicted; choose one of: NONE, ALL, or "tag|tag!...!tag". Note that these tags refer to the verbose name (_V datatype) of the datafield.
- PRINT_SCHEMA**
Useful for the Graph datatype, as in "-PRINT_SCHEMA Graph".
- PRINT_STEREO**
Use with 3-D data for stereo pairs.
- PRINT_TEXT**
Specify which datatypes are to be shown textually; choose one of NONE, ALL, or "tag|tag!...!tag". Note that data such as SMILES can be both depicted and printed as text.

3.1 Treetops Examples

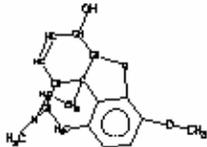
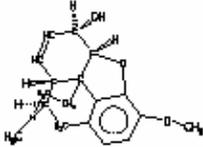
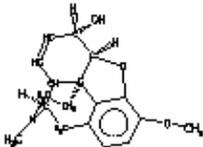
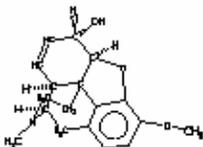
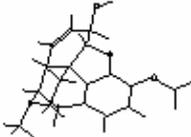
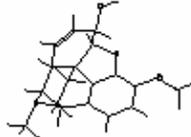
Let's assume for these examples that an FDT file has been produced for the compound codeine by using the program Thorlookup and extracting data from an available database. Here is the FDT file (with tab's shown as

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"=>"):

```
SMILES=>COc1ccc2CC3C4C=CC(O)C5Oc1c2C54CCN3C
=>Remark=>This data excerpted from Spresi93 and Pomona93c.
=>SPRESI Registry Number=>126226-200
=>SPRESI Registry Number=>126226-209
=>=>Isomer=>COc1ccc2C[C@H]3[C@@H]4C=CC(O)C5Oc1c2[C@]54CCN3C
=>SPRESI Registry Number=>126226-401
=>=>Isomer=>COc1ccc2C[C@@H]3[C@H]4C=C[C@H](O)[C@@H]5Oc1c2C54CCN3C
=>SPRESI Registry Number=>126226-602
=>=>Isomer=>COc1ccc2C[C@@H]3[C@@H]4C=C[C@@H](O)[C@@H]5Oc1c2C54CCN3C
=>SPRESI Registry Number=>126226-707
=>=>Isomer=>COc1ccc2CC3C4C=C[C@@H](O)[C@H]5Oc1c2[C@]54CCN3C
=>SPRESI Registry Number=>126226-803
=>=>Isomer=>COc1ccc2C[C@@H]3[C@@H]4C=C[C@H](O)[C@@H]5Oc1c2C54CCN3C
=>SPRESI Registry Number=>126226-811
=>=>Isomer=>COc1ccc2C[C@@H]3[C@@H]4C=CC(O)C5Oc1c2[C@]54CCN3C
=>POMONA Name=>PREINE
=>=>Conformation=>-204.02=>Name=>PREINE=>3D-coords=>5.12,0.49,0.33,etc.,
etc.,-3.77,-2.52,0.58=>Source=>
=>=>Orientation=>CONCORD293=>TR matrix=>0.45545,-0.47645,0.65594,
2.98298,-0.14266,-2.67709
```

If we use Treetops in its default mode to print this file, we will obtain:

SMILES		
Remark	This data excerpted from Spresi95 and Medchem95c.	
SPRESI Registry Number	0126226-120	
Isomer		
SPRESI Registry Number	0126226-217	
Isomer		
SPRESI Registry Number	0126226-313	
Isomer		
Pomona Name	CODEINE	
Conformation	-203.40	
Name	Med95	
3D-coords		
Source	CON301 	

4. Prado

Prado is used for printing depictions of structures. The online help text is obtained with "prado -help":

```
% prado -help
```

```
prado 4.71, Daylight CIS Inc. -- SYNTAX SUMMARY
```

```
Print depictions from SMILES
```

```
Usage: prado [options] < in.[smi|tdt] > out.ps
or: prado [options] in.[smi|tdt] > out.ps
or: prado [options] in.[smi|tdt] out.ps
```

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```
or: prado -help          (show this summary)
or: prado -notes        (show release notes)
or: prado -options      (show option summary)
or: prado -settings     (show current settings)
```

The options are listed by entering "prado -options":

```
% prado -options
prado 4.71 Daylight CIS Inc. -- OPTION SUMMARY

Print depictions from SMILES

Usage: prado [options] < in.[smi|tdt] > out.ps
or: prado [options] in.[smi|tdt] > out.ps
or: prado [options] in.[smi|tdt] out.ps

Page formatting options:
-DEPICT_SUPPRESS_LABELS [TRUE|FALSE]
-PRINT_BINDER [NONE|LEFT|TOP|LEFTRIGHT|TOPBOTTOM]
-PRINT_BOLDWIDTH [THIN|NORMAL|WIDE|EXTRAWIDE]
-PRINT_COLORMODE [BOW|WOB|COW|COB]
-PRINT_COLUMNS <number of columns in depiction grid>
-PRINT_FOOTER [NONE|STANDARD]
-PRINT_HINTS [NONE|FROMTO]
-PRINT_LABELSIZE <footer font size in points>
-PRINT_LANGUAGE PS|EPS
-PRINT_LINEWIDTH [THIN|NORMAL|WIDE|EXTRAWIDE]
-PRINT_MARGINS [BLEED|MINIMAL|NARROW|NORMAL|WIDE|HUGE]
-PRINT_NAMETAG <.tdt tag to appear as name>
-PRINT_ORIENT [TALL|WIDE]
-PRINT_PAGELIMIT 100
-PRINT_PAPER [USLETTER|USLEGAL|USTABLOID|A3|A4|A5|B5|
COMPUTER|FANFOLD]
-PRINT_ROWS <number of rows in depiction grid>
-PRINT_SHADOW [TRUE|FALSE]
-PRINT_SMARTS NONE or SMARTS to highlight
-PRINT_TITLE NONE or "any string"
-PRINT_TITLESIZE <title font size in points>
```

The Prado options are described more fully below.

PAGE FORMATTING OPTIONS:

DEPICT_SUPPRESS_LABELS

Suppress atom labelling for chains, one of [TRUE | FALSE].

PRINT_BINDER

If the pages printed are to be bound, appropriate spacing can be specified. Select one of: [NONE | LEFT | TOP | LEFTRIGHT | TOP | BOTTOM].

PRINT_BOLDWIDTH

Specify the width of the lines used for highlighted parts of depictions, one of [THIN | NORMAL | WIDE | EXRTAWIDE].

PRINT_COLORMODE

Specify black-on-white, white-on-black, color-on-white, or color-on-black, one of [BOW | WOB | COW | COB].

PRINT_COLUMNS

Number of columns in depiction grid.

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PRINT_FOOTER

Print footer information and page number; one of [STANDARD | NONE].

PRINT_LABELSIZE

Size of font used for labels.

PRINT_LANGUAGE

Format of output file, one of [PS | EPS]. PS (PostScript) is used to print directly, EPS (Encapsulated PostScript) is often used to include graphics within another document.

PRINT_LINEWIDTH

Specify the width of the lines used for depictions, one of [THIN | NORMAL | WIDE | EXRTAWIDE].

PRINT_MARGINS

One of: [BLEED | MINIMAL | NARROW | NORMAL | WIDE | HUGE].

PRINT_NAMETAG

Specify which datatype from the TDT file should be used to title each depiction (use brief tag).

PRINT_ORIENT

One of [TALL | WIDE].

PRINT_PAGELIMIT

Maximum number of pages to print.

PRINT_PAPER

Paper size; choose one of [USLETTER | USLEGAL | USTABLOID | A3 | A4 | A5 | B5 | COMPUTER | FANFOLD].

PRINT_ROWS

Number of rows in depiction grid.

PRINT_SHADOW

Shadow-style boxes desired? Choose TRUE or FALSE.

PRINT_SMARTS

Specifying a SMARTS with this option will highlight atoms of the hit SMARTS in the input structures if there is a hit.

PRINT_TITLE

Title for output document; appears at the top of each page.

PRINT_TITLEFONT

Font for title.

PRINT_TITLESIZE

Size of font used in title, in points.

4.1 Prado Examples

Here's a sample SMILES file which we will use as input for Prado:

```
NCCc1ccc(O)c(O)c1 DOPAMINE
CN1C(=O)N(C)C(=O)C(N(C)C=N2)=C12 CAFFEINE
CCN(CC)C(=O)C1CN(C)C2CC3=CNc(ccc4)c3c4C2=C1 LSD
N12CCC36C1CC(C(C2)=CCOC4CC5=O)C4C3N5c7cccc76 STRYCHNINE
OCC1OC(O)C(O)C(O)C1O GLUCOSE
Nc1cc(nc(N)n1=O)N2CCCC2 MINOXIDIL
C123C5C(O)C=CC2C(N(C)CC1)Cc(ccc4O)c3c4O5 MORPHINE
N1N([Hg-][O+]=C1N=Nc2cccc2)c3cccc3 MERCUROUS CARBAZONE COMPLEX
NC(Cc1c[nH]c2cccc12)C(O)=O TRYPTOPHAN
COC(=O)COc1cccc1 PHENOXYACETICACID,METHYLESTER
[C1-].[C1-].NC(=O)c2cc[n+](COC[n+]1cccc1C=NO)cc2 HI-6
CCCN(CCC)C1Cc2c[nH]c3ccc(OC)c(C1)c23 BAYR1531
CN1C(=O)CN=C(c2cccc2)c3cc(C1)ccc13 DIAZEPAM
CC12CCC3C(CCC4=CC(=O)CCC34C)C2CCC1O TESTOSTERONE
```

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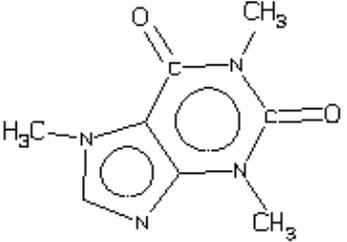
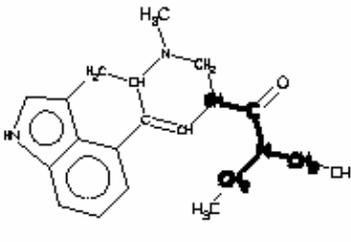
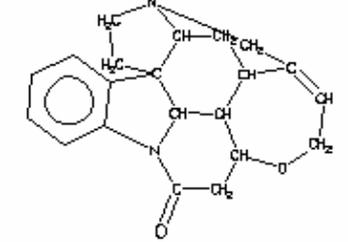
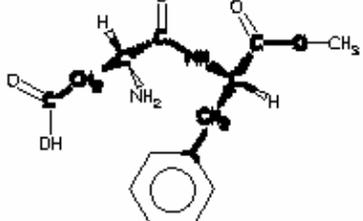
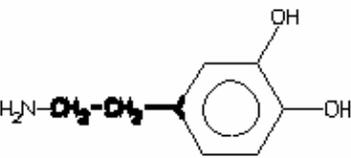
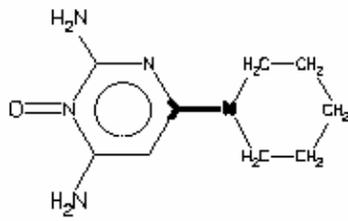
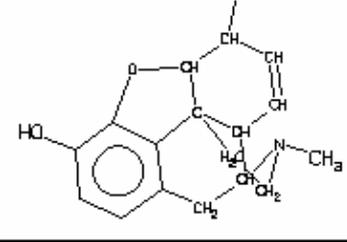
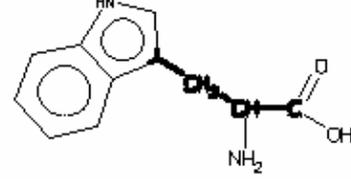
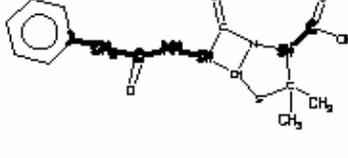
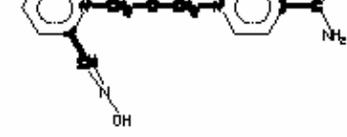
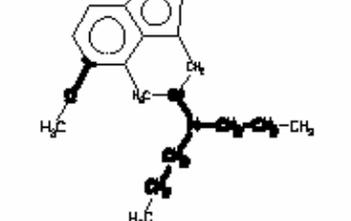
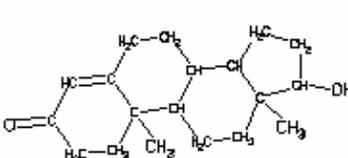
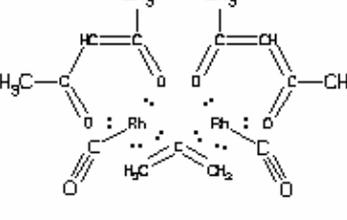
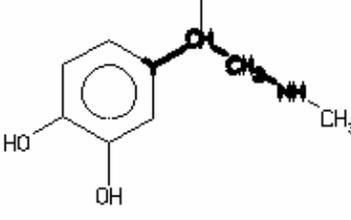
CC4=O[Rh]1([CH2]=C12=[CH2][Rh]23(O=C(=[CH]=C(=O3)C)C)C#O(O=C(=[CH]4)C)C#O AACRHC

Here's what we get when we print with Prado in its default mode:

<p>Caffeine</p>	<p>LSD</p>	<p>Strychnine</p>
<p>Aspartame</p>	<p>Dopamine</p>	<p>Minoxidil</p>
<p>Morphine</p>	<p>Tryptophan</p>	<p>Benzylpenicillin</p>
<p>HI-6</p> <p>α</p> <p>α</p>	<p>BAYR1531</p>	<p>Testosterone</p>
<p>AACRHC</p>	<p>Adrenalin</p>	<p>Zantac</p>

If we specify a SMARTS to highlight, we also see the effect of increased line width. Here the SMARTS are highlighted with "EXTRAWIDE" lines:

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<p>Caffeine</p> 	<p>LSD</p> 	<p>Strychnine</p> 
<p>Aspartame</p> 	<p>Dopamine</p> 	<p>Minoxidil</p> 
<p>Morphine</p> 	<p>Tryptophan</p> 	<p>Benzylpenicillin</p> 
<p>HI-6</p>  <p>α</p> <p>α</p>	<p>BAYR1531</p> 	<p>Testosterone</p> 
<p>AACRHC</p> 	<p>Adrenalin</p> 	<p>Zantac</p> 

5. Tablet

Tablet is used for printing tables representing Merlin hitlists. Here's the online help text, obtained by entering "tablet -help":

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```
% tablet -help
tablet 4.71 Daylight CIS Inc. -- SYNTAX SUMMARY
Convert tab-delimited file to PostScript file with depictions
Usage:  tablet [options] in.tab > out.ps
or:    tablet [options] in.tab out.ps
or:    tablet -help                (show this summary)
or:    tablet -notes                (show release notes)
or:    tablet -options              (show option summary)
or:    tablet -settings             (show current settings)
```

Here's the option list obtained by entering "tablet -options".

```
% tablet -options
tablet 4.71 Daylight CIS Inc. -- OPTION SUMMARY

Convert tab-delimited file to PostScript file with depictions
Usage:  tablet [options] < in.tab > out.ps
or:    tablet [options] in.tab > out.ps
or:    tablet [options] in.tab out.ps

Options:
-DEPICT_SUPPRESS_LABELS  [TRUE|FALSE]
-PRINT_BINDER            [NONE|LEFT|TOP|LEFTRIGHT|TOPBOTTOM]
-PRINT_BOLDWIDTH        [THIN|NORMAL|WIDE|EXTRAWIDE]
-PRINT_COLORMODE        [BOW|WOB|COW|COB]
-PRINT_DATAFONT         "Helvetica"
-PRINT_DATASIZE         <size of font used for data, points>
-PRINT_FOOTER           NONE|STANDARD
-PRINT_LABELFONT        "Helvetica-BoldOblique"
-PRINT_LABELSIZE        <size of font used for labels, points>
-PRINT_LANGUAGE         PS|EPS
-PRINT_LINEWIDTH        [THIN|NORMAL|WIDE|EXTRAWIDE]
-PRINT_MARGINS          [BLEED|MINIMAL|NARROW|NORMAL|WIDE|HUGE]
-PRINT_ORIENT           [TALL|WIDE]
-PRINT_PAPER            [USLETTER|USLEGAL|USTABLOID|A3|A4|A5|B5|
                        COMPUTER|FANFOLD]
-PRINT_PAGELIMIT        <max number of pages to print>
-PRINT_PICTSIZE         <height of pictures in points>
-PRINT_SMARTS           [NONE|SMARTS to highlight]
-PRINT_SMILES           [TEXT|DEPICTION]
-PRINT_TITLE            "any string" or NONE
-PRINT_TITLEFONT        "Helvetica-Bold"
-PRINT_TITLESIZE        <size of font used for title, points>
```

The tablet options are described more fully below.

OPTIONS:

DEPICT_SUPPRESS_LABELS [TRUE | FALSE]

Suppress atom labelling for chains, one of [TRUE | FALSE].

LICENSEDATA file

The Daylight license file. Default: /usr/local/daylight/dy_license.dat.

PRINT_BINDER [NONE | LEFT | TOP | LEFTRIGHT | TOPBOTTOM]

Paper margin to get extra room for binding. Default NONE.

PRINT_BOLDWIDTH [THIN | NORMAL | WIDE | EXTRAWIDE]

Bold graphic line width (shows foreground, substructure). Default NORMAL.

PRINT_COLFORMS char[char...]

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A string defining the format to be used for each column. Each character in this string corresponds to the format of one column. If there are more columns than characters in the string, the value of the last format character is used for all remaining columns. The default value is "G", which applies G to all columns. The format characters are:

- C .. center ... equal space on left and right
- D .. decimal .. line up (first) decimal points
- G .. general .. guess R if all digits, J if space, else L
- J .. justify .. line up left and right by expanding spaces
- L .. left line up left extent, right is ragged
- R .. right line up right extent, left is ragged
- S .. SMILES ... treat as SMILES

PRINT_COLORMODE [BOW | WOB | COW | COB]

Printing color mode [Black | White | Color] On [Black | White]. Default BOW (Black-On-White).

PRINT_FOOTER [STANDARD | NONE]

Print footer information and page number. Default is STANDARD.

PRINT_LANGUAGE [PS | EPS]

Output language (PS = PostScript, EPS = Encapsulated PostScript)

PRINT_LINEWIDTH [THIN | NORMAL | WIDE | EXTRAWIDE]

Regular Graphic line width (shows background, borders, structures). Default THIN.

PRINT_MARGINS [BLEED | MINIMAL | NARROW | NORMAL | WIDE | HUGE]

Basic print margins. Default NORMAL.

PRINT_ORIENT [TALL | WIDE]

Paper orientation for printing. Default TALL.

PRINT_PAPER paper

Choices are: USLETTER, USLEGAL, USTABLOID, A3, A4, A5, B5, COMPUTER, FANFOLD.
Default USLETTER.

PRINT_PAGELIMIT N

Limit number of pages of output to produce (0 means no limit). Default is 100.

PRINT_PICTSIZE size

Size of embedded pictures in printed output (see -PRINT_DEPICT, above). Default: 72 (points).

PRINT_SMILES [TEXT | DEPICTION]

Given the choice, should SMILES be printed as text or picture? Default: DEPICTION.

PRINT_SMARTS smart

A SMARTS string, if given, causes that substructure to be highlighted in every structure drawn.
Default is "NONE" (no highlighting).

PRINT_DATAFONT font

Font used to print data. Default: Helvetica.

PRINT_DATASIZE size

Size of font used to print data. Default: 10 (points).

PRINT_LABELFONT font

Font used to print labels. Default: Helvetica-BoldOblique.

PRINT_LABELSIZE size

Size of printed labels. Default: 10.

PRINT_TITLE title

Title for printed output. Default NONE (no title).

PRINT_TITLEFONT

Font used to print title. Default Helvetica-Bold.

PRINT_TITLESIZE

Font size used to print title. Default 14.

PRINT_TITLEPICT TRUE | FALSE

Print PRINT_TITLE as a depiction? Default FALSE.

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PRINT_TPICTSIZE

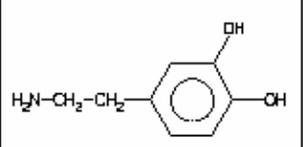
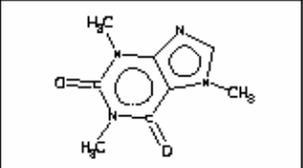
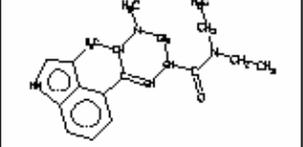
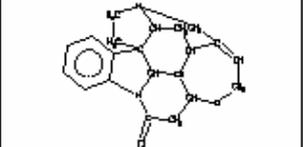
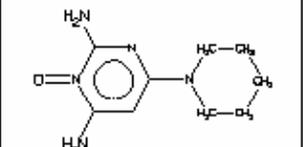
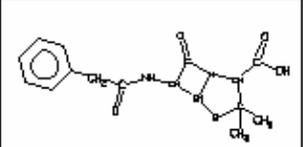
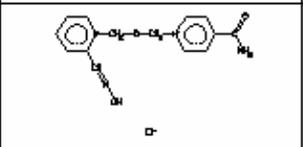
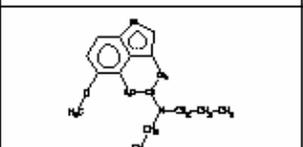
The size of the depicted title. Only has effect if PRINT_TITLEPICT is TRUE. Default: 144 (points).

Tab files are normally produced by Merlin via the 'Save hitlist as .TAB file...' command. Here's a sample (with tab's shown as "=>"):

```
SMILES=>CAS No=>Local name=>Activity=>CLOGP
NCCc1ccc(O)c(O)c1=>51-61-6=>DOPAMINE=>ADRENERGIC=>-0.051
Cn1cnc2n(C)c(=O)n(C)c(=O)c12=>58-08-2=>CAFFEINE=>STIMULANT=>0.056
CCN(CC)C(=O)C1CN(C)C2Cc3c[nH]c4cccc(C2=C1)c34=>50-37-3=>
"LYSERGICACID,DIETHYLAMIDE"=>HALLLUCINOGENIC(5-HT2-AGONIST)=>2.498
O=C1CC2OCC=C3CN4CCC56C4CC3C2C6N1c7cccc75=>57-24-9=>STRYCHNINE=>
CNS STIMULANT (VET)=>-0.365
OCC1OC(O)C(O)C(O)C1O=>50-99-7=>GLUCOSE=>" "=>-3.529
Nc1cc(nc(N)n1=O)N2CCCC2=>38304-91-5=>MINOXIDIL=>ANTIHYPERTENSIVE=>1.068
CN1CCC23C4Oc5c3c(CC1C2C=CC4O)ccc5O=>57-27-2=>MORPHINE=>
ANALGESIC (NARCOTIC)=>0.182
N1N([Hg-][O+]=C1N=Nc2cccc2)c3cccc3=>" "=>MERCUROUS CARBAZONE COMPLEX=>" "=>" "
```

Here's the Tablet output we obtain with the default options:

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SMILES	Local name	CAS No	Activity	CLOGP
	DOPAMINE	51-61-6	ADRENERGIC	0.019
	CAFFEINE	58-08-2	STIMULANT	-0.251
	LYSERGICACID,DIETHYL AMIDE	50-37-3	HALLUCINOGENIC (5-HT2-AGONIST)	2.488
	STRYCHNINE	57-24-9	CNS STIMULANT (VET)	-0.305
	MINOXIDIL	38304-91-5	ANTIHYPERTENSIVE, ANTIALOPECIA	1.39
	BENZYLPENICILLIN	61-33-6	ANTIBACTERIAL	1.683
	HI-6	34433-31-3		
	BAY R 1531		ANTIDEPRESSANT, SEXUAL STIMULANT	3.687

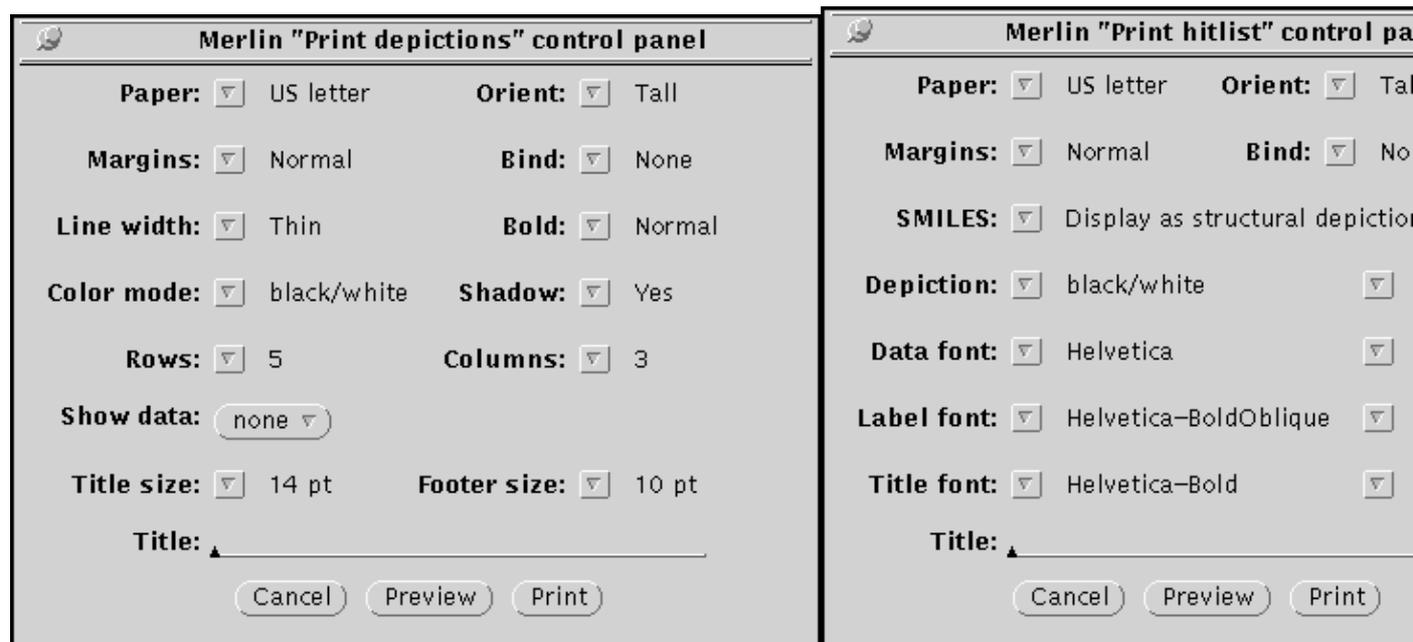
6. Printing from Thor and Merlin

Treetops style output can also be printed directly from the Thor application program, and Prado and Tablet style output can be printed directly from the Merlin program.

Thor uses Treetops to print a Thor Data Tree (TDT) from the TDT Widget. After displaying the TDT Widget with the 'Show Datatree' button, the 'Print', button becomes available. Pressing this button results in three

things happening: (1) The TDT is sent to a Treetops for conversion to a PostScript file located in a directory specified by option PRINT_DIRECTORY, (2) A print command is performed as specified by the Daylight option: PRINT_PS_MONO_ZAP_CMD or PRINT_PS_COLOR_ZAP_CMD (where the choice is determined by option PRINT_COLOR_MODE), and (3) the temporary PostScript file is deleted.

Merlin uses Tablet and Prado in an analogous way. From the 'File' menu on the Merlin window, select either 'Print Hitlist...' for Tablet style output, or 'Print Depictions...' for Prado style output. One of the following two control panel will appear:



Merlin allows full control over the printed output via these panels, which are really just an interface for setting any of the Tablet and Prado options. Similarly to Thor, when a Merlin print button is pressed, a temporary TAB or SMILES file is produced for the current hitlist, this file is processed by Tablet or Prado, and the resulting temporary PostScript file is printed.

Although Thor offers less interactive control over the printed output, in fact all of the options available to Treetops can be set for Thor. However, they must be set before starting the Thor client program. Similarly, Prado and Tablet options can be set prior to starting Merlin. These options can be set on the Thor/Merlin command line, or in Daylight option-specification files, or via local environment variables. For more help on setting options, see the Daylight Administrator's Guide.

Appendix 1: Printing PostScript Files

Printer Setup for Daylight Software 4.x

Daylight Software version 4.x provides the capability to print text and graphics for chemical structures and data directly from the applications, or via PostScript files. However, for Daylight's printing capabilities to work, the computer and printer must be correctly configured. In general, this will mean configuring the system to print a PostScript file with the command "lpr foo.ps".

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The procedure for setting up a computer and printer to print a PostScript file will vary from machine to machine. The following summary is intended to help with getting started, not to be a complete set of instructions.

- Printing a PS file requires a PS interpreter, either loaded as software on the computer, or, more typically, built into the printer, a PS printer such as the Apple LaserWriter.
- The printer must be connected to the computer by either a serial, parallel, or network connection, depending on the capabilities of the machine and printing software. A "network" printer may be attached directly to a network, or may be attached via a printserver host.
- SunOS machines need to have "NewsPrint" software loaded to print proficiently. SGI/IRIX machines do not need additional software, but to talk to lpr-spooling daemons on other machines with Berkeley-style UNIX, the "eoe2.sw.bsdlpr BSD Line Printer Spooling Utilities" software must have been loaded from the system disk. Otherwise, the ATT-style lp-spooling system can be used on SGI/IRIX machines.
- UNIX machines require that each printer have an entry in /etc/printcap. Refer to your system documentation for the specific entries needed.
- In many typical situations, one printer will serve several hosts and users. If this is an Apple LaserWriter, for example, this printer will be considered a "serial printer" by the host to which it is connected (the printserver), and a "network printer" by the other hosts. Each machine will have an entry in its /etc/printcap describing this printer. Alternately, it may be possible to use "rsh" to avoid the need to define a printer on a given machine. For example, the command: "cat foo.ps | rsh crawdad lpr - " may work to print from a host with no printer defined, via printserver "crawdad".

Appendix 2: The FDT File Format

The "FDT" file format (Formatted Data Tree) was introduced by Daylight to support the Daylight PrintPackage, although it may well find other uses.

Unlike the TDT format, which contains abbreviations and indirect references which rely on other files or databases for their meaning, the FDT format contains verbose datatype tags, and expanded indirect data. Therefore, the FDT format is self-contained.

Tabs are used as delimiters, both to separate data-tags and datafields, and to signify the tree-depth of a line in the FDT file. Each line in the FDT file represents one datatype, and if a datatype consists of multiple fields, the line goes <datatag><tab><value><tab><datatag2><value><tab><datatag3><value>, etc.

See the Treetops section of this manual for an example.

Appendix 3: The TAB File Format

The TAB format is now also defined as the input format for Tablet. The TAB format is written by Merlin in saving hitlists.

The TAB format represents an RxC grid of R rows and C columns, as is displayed on Merlin's main canvas. There are R+1 lines in the TAB file, with the first line containing the column titles. This format is equivalent to certain common spreadsheet file formats, which can enable data transfer.

See the Tablet section of this manual for an example.

Appendix 4: Daylight PRINT Options

In addition to the Daylight options listed herein for the Treetops, Prado, and Tablet programs, there are a few Daylight options used by other application programs to actually print an output PostScript file, and perform other related duties. These options are listed below:

PRINT_DIRECTORY

The directory for temporary print files.

PRINT_EXECUTE_FG_CMD

Command used to execute print program synchronously. This is used when the next action is dependent on this command.

PRINT_EXECUTE_BG_CMD

Command used to execute a command in the background. This is used when the next action is not dependent on this command, for example a delete command or send-to-printer command.

PRINT_DELETE_CMD

Command used to delete temporary print file, such as an FDT or TAB file.

PRINT_PS_MONO_CMD

Command used to print a PS file and not delete it.

PRINT_PS_MONO_ZAP_CMD

Command used to print a PS file and delete it (this is the default).

PRINT_PS_COLOR_CMD

Command used to print a color PS file and not delete it.

PRINT_PS_COLOR_ZAP_CMD

Command used to print a color PS file and delete it.

PRINT_PS_VIEW_CMD

Command used to view a PS file on the display (the system must have software to do this) and not delete it.

PRINT_PS_VIEW_ZAP_CMD Command used to view a PS file on the display (the system must have software to do this) and delete it.