NAME

SDFilesToHTML.pl - Generate HTML table file(s) from SDFile(s)

SYNOPSIS

SDFilesToHTML.pl SDFiles(s)...

SDFilesToHTML.pl [-a, --align left | center | right,[top | middle | bottom]] [-b, --border borderwidth] [--cellpadding padding] [--cellspacing spacing] [--cmpddatafield "fieldlabel,[label,position,alignment]"] [--datafields "fieldlabel,[fieldlabel]..." | Common | All] [--footer string] [-d, --displaylinks top | bottom | both] [--displaylinksinfo compound | table | both] [-h, --help] [--headeralign left | center | right,[top | middle | bottom]] [--headercolor "#RRGGBB"] [--highlight "fieldlabel,datatype,criterion,value,[fieldlabel,datatype,criterion,value,...]"] [--highlightcolor "#RRGGBB,#RRGGBB"] [--highlightstyle text | background] [-m, --mode plain | shade | highlight | shadedhighlight | structuresonly | shadedstructuresonly] [-n, --numcmpds number] [-o, --overwrite] [-r, --root rootname] [-s, --structure display | link] [--strlinkmode plain | shaded] [--strlinknavigation yes | no] [--strlinkshadecolor "#RRGGBB"] [--strlinktitle string] [--strlinktitledisplay yes | no] [--strlinktype href | button] [--strviewertype Chem3DActiveX | ChemDrawActiveX | ChemDrawPlugIn | Chime | JME | Jmol | MarvinView | ViewerActiveX] [--strviewerconfig codebase[,archive,code]] [--strviewerparams "name=value [name=value ...]"] [--strviewerembed direct | javascript] [--strviewerjsfile javascriptfilename] [--strtablesize "numrows,numcols"] [--stylesheet old | new | none] [--stylesheetname filename] [--shadecolor "#RRGGBB,#RRGGBB"] [-t, --title string] [--titledisplay yes | no] [-w, --workingdir dirname] SDFiles(s)...

DESCRIPTION

Generate HTML file(s) from *SDFile(s)*. The HTML file(s) contain data tables and appropriate navigational links to view other tables; navigational links are also provided on compound HTML pages. These files can be generated for local viewing or deployment on a web server. A variety of options are provided to control style and appearance of tables. And for viewing structures, options are available to use any one of these viewers: Chem3DActiveX, ChemDrawActiveX, ChemDrawPlugIn, Chime, Jmol, JME, MarvinView, or ViewerActiveX. Jmol is the default structure viewer and it is also distributed along with this package; however, to use any other supported viewers, make sure it's available in your environment.

Multiple *SDFile(s)* names are separated by space. The valid file extensions are *.sdf* and *.sd*. All other file names are ignored. All the SD files in a current directory can be specified either by **.sdf* or the current directory name.

OPTIONS

`-a, --align` *left | center | right,[top | middle | bottom]*

Horizontal and vertical alignment for table rows except for header row which is specified using `--headeralign` option. Possible horizontal alignment values: *left, center, or right*. Possible vertical alignment values: *top, middle, or bottom*.

Default values: *left,middle*

`-b, --border` *borderwidth*

Table border width. Default value: 1 for *plain* and *highlight* mode; 0 for *shade* and *shadedhightlight* mode. Zero indicates no border.

`--cellpadding` *padding*

Table cell padding. Default value: *2*.

`--cellspacing` *spacing*

Table cell spacing. Default value: *1*.

`--cmpddatafield` *fieldlabel,[label,position,alignment]*

This value is mode specific. It indicates data field value to be displayed with the structure along with its label, position and alignment during *structuresonly | shadedstructuresonly* value of `-m, --mode` option. Possible values: feldlabel - valid data field label; label - yes or no; position - *top or bottom*; alignment - *left, center, or right*. Default: *none,no,bottom,center*. Example:

```
MolWt,no,bottom,middle
```

`--cmpddatafield` option value is also linked to compound summary page.

`--datafields` *"fieldlabel,[fieldlabel]..." | Common | All*

Data fields to display in HTML table(s). Possible values: list of comma separated data field labels, data fields common to all records, or all data fields. Default value: *All*. Examples:

```
ALogP,MolWeight,EC50
"MolWeight,PSA"
```

--footer *string*

Text string to be included at bottom of each HTML file. Default: none.

-d --displaylinks *top* | *bottom* | *both*

Specify where to display navigation links in each HTML file for accessing all other HTML files. Possible values: *top, bottom, or both*. Default: *both*. This option is only valid during multiple HTML files generation for an input file.

--displaylinksinfo *compound* | *table* | *both*

Control display of additional information along with navigational links: Showing compound n of m is displyed for compound and showing table n of m for table. Possible values: *compound* | *table* | *both*. Default: *both*. This option is only valid during multiple HTML files generation.

-h, --help

Print this help message.

--headeralign *left* | *center* | *right,[top* | *middle* | *bottom*

Horizontal and vertical alignment for table header rows. Possible horizontal alignment values: *left, center, or right*. Possible vertical alignment values: *top, middle, or bottom*.

Default values: *center,middle*

--headercolor *#RRGGBB*

Color used to fill background of table header row containing column labels represented as a hexadecimal string. Default value: None for -m, --mode option value of *plain* and *#ccccff*, light blue, for others.

--highlight *"fieldlabel,datatype,criterion,value,[fieldlabel,datatype,criterion,value,...]"*

Highlighting methodology used to highlight various SDFile(s) data field values in HTML file(s). Same set of quartets values are applied to all SDFile(s).

Input text contains these quartets: *fieldlabel,datatype,criterion,value,...*. Possible datatype values: *numeric or text*. Possible criterion values: *le, ge, or eq*. Examples:

```
"MolWt,numeric,le,450"
"MolWt,numeric,le,450,LogP,numeric,le,5"
Name,text,eq,Aspirin
```

--highlightcolor *"#RRGGBB,#RRGGBB"*

Colors used to highlight column values during *highlight* and *shadedhightlight* mode represented as hexadecimal strings.

For --highlighstyle option values of *text* and *background*, these colors represent text or background colors respectively. For a specific column, first color string is used for values which meet criterion indicated by --highlight option; the second color is used for rest of the values.

Default values for *background* --highlightstyle: *"#0fff0f,#ff0f0f"*. And default values for *text* --highlightstyle: *"#0fbb0f,#ff0f0f"*. Hexadecimal strings for both --highlightstyle colors correspond to *reddish* and *greenish*.

--highlightstyle *text* | *background*

This value is mode specific. It indicates highlight style used to differentiate column values which meet a specified criterion in --highlight option. Possible values: *text or background*. Default: *background*.

-m, --mode *plain* | *shade* | *highlight* | *shadedhighlight* | *structuresonly* | *shadedstructuresonly*

Specify how to generate HTML table(s): plain tables with line borders, background of alternate rows filled with a specified color, column values highlighted using a specified criteria, combination of previous two styles, tables containing only structures, or tables containing only structures with filled background of alternate rows.

Possible values: *plain, shade, highlight, shadedhighlight, structuresonly, or shadedstructuresonly*. Default: *shade*.

-n, --numcmpds *number*

Maximum number of compounds per table. Default value: *15* for tables with structures and *50* for tables with links to structures. Use 0 to put all compounds into one table. For SDFile(s) with more than maximum number of specified compounds, multiple HTML tables, with appropriate navigation links, are created.

-o, --overwrite

Overwrite existing files.

-r, --root *rootname*

New file or directory name is generated using the root: <root>.html or <root>-html. Default new file name: <InitialSDFileName>.html. Default directory name: <InitialSDFileName>-html.

For SDFile(s) with more than maximum number of specified compounds per table, this directory tree is generated using <Name> where <Name> corresponds to <root> or <InitialSDFileName>: Top dir - <Name>-html; Sub dirs - html and mols. <Top dir> contains <Name>.html and <Name>.css files and <sub dir> html conatins various <Name>Lines<Start>To<End>.html files; <sub dir> mols is created as needed and contains MOL files.

This option is ignored for multiple input files.

-s, --structure *display* | *link*

Structure display control: display structures in a table column or set up a link for each structure which opens up a new HTML page containing structure and other appropriate information. Possible values: *display or link*. Default value: *display*

--strlinkmode *plain* | *shaded*

Specify how to display compound HTML page: plain or background of data field field labels is filled with a specified color. Possible values: *plain or shad*. Default value: *plane*.

Structure viewer background color is white. Use --strviewerparams option to change default behavior of structure viewers.

--strlinknavigation *yes* | *no*

Display navigation links to other compounds in compound HTML page. Possible values: *yes or no*. Default value: *yes*.

--strlinkshadecolor *"#RRGGBB"*

This value is --strlinkmode specific. For *shade* value of --strlinkmode option, it represents colors used to fill background of data field labels.

Default value: *"#e0e9eb"* - it's a very light blue color.

--strlinktitle *string*

Title for compound HTML page. Default value: *Compound Summary*.

--strlinktitledisplay *yes* | *no*

Display title for compound HTML page. Possible values: *yes or no*. Default value: *no*.

--strlinktype *href* | *button*

Type of structure link. Possible values: *href or button*. Default: *href*.

--strviewertype *Chem3DActiveX* | *ChemDrawActiveX* | *ChemDrawPlugIn* | *Chime* | *JME* | *Jmol* | *MarvinView* | *ViewerActiveX*

Structure viewer supported for viewing structures. Possible values: *Chem3DActiveX, ChemDrawActiveX, ChemDrawPlugIn, Chime, JME, Jmol, MarvinView, or ViewerActiveX*. Default value: *Jmol*.

Assuming you have access to one of these viewers on your machine, you are all set to use this script. Otherwise, visit one of these web sites to download and install your favorite viewer:

```
accelrys.com: Viewer ActiveX 5.0
cambridgesoft.com: Chem3DActiveX 8.0, ChemDrawActiveX 8.0,
                   ChemDrawPlugIn
chemaxon.com: MarvinView applet
mdli.com: Chime plug-in
jmol.sourceforge.net: JmolApplet V10
molinspiration.com: JME applet
```

The default viewer, JmolApplet V10, is distributed with MayaChemTools package. Earlier versions of JmolApplet are not supported: due to applet security issues related to reading files, this script uses in-line loading of MOL files and this option doesn't exist in earlier version of JmolApplet.

--strviewerconfig *codebase[,archive,code]*

Configuration information for structure viewers. This option is only valid for structure viewers which are applets: Jmol, JME and MarvinView. For other viewer types available via --strviewertype option - MDL Chime, ChemDrawActiveX, ChemDrawPlugIn, and Chem3DActiveX - this value is ignored.

Input text format: *codebase[,archive,code]*. For an applet viewer, *codebase* must be specified; *archive* and *code* values are optional. Here are default *archive* and *codebase* values for various applets: Jmol - JmolApplet, JmolApplet.jar; JME - JME, JME.jar; MarvinView: MView, marvin.jar

For local deployment of HTML files, *codebase* must correspond to a complete path to the local directory containing appropriate *archive* file and the complete path is converted into appropriate relative path during generation of HTML files.

By default, *codebase* value of <this script dir>/../lib/Jmol is used for *Jmol* applet viewer, and HTML file(s) are generated for local deployment; however, you can specify any supported applet viewer and generate HTML file(s) for deploying on a web server.

For deploying the HTML file(s) on a web server, specify a valid *codebase* directory name relative to <WWWRootDir>. Example when JME archive file, JME.jar, is available in */jme* directory on the web server:

```
/jme
```

For local deployment of HTML file(s), specify a complete *codebase* directory name. Example when JmolApplet archive file, JmolApplet.jar, is present in <JMOLROOT> directory:

```
<JMOLROOT>
```

In addition to *codebase*, you can also specify *archive* file name. Example for web deployment:

```
"/jme,JME.jar"
"/jme"
```

Example for local deployment:

```
"<JMEROOT>,JME.jar"
"<JMEROOT>"
```

--strviewerparams *"name=value [name=value ...]"*

Parameters name and value pairs for structure viewers. These name and value pairs are used to control the appearance and behavior of structure viewers in tables and compound HTML page during *link* value for -s --structure option.

The parameter names, along with their values, are just passed to each structure viewer in appropriate format without checking their validity. Check documentation of appropriate structure viewers to figure out valid parameter names.

Input text format: *name=value name=value ...* Example:

```
"width=250 height=170"
```

Default for all structure viewers: *width=250 height=170* for displaying structures in tables, and *strlinkwidth=500 strlinkheight=295* for compound HTML page during *link* value for -s --structure option.

Default background color for all structure viewers: same as --shadecolor value for displaying structures in tables and *strlinkbgcolor=#ffffff* for compound HTML page; however, explicit specification of background color in this option overrides default value. To use black background for structures in tables and compound HTML page, specify *bgcolor=#000000* and *strlinkbgcolor=#000000* respectively. Keep this in mind: Some structure viewers don't appear to support background color parameter.

Additional structure viewer specific default values:

```
Chem3DActiveX: "displaytype=Ball&Stick rotationbars=false
                moviecontroller=false"
ChemDrawActiveX: "ViewOnly=1 ShrinkToFit=1 ShowToolsWhenVisible=1"
ChemDrawPlugIn: "type=chemical/x-mdl-molfile ViewOnly=1
                 ShrinkToFit=1 ShowToolsWhenVisible=1"
Chime: "display2d=true"
```

```
JME: "options=depict"
Jmol: "progressbar=true progresscolor=#0000ff boxbgcolor=#000000
       boxfgcolor=#ffffff script="select *; set frank off;
       wireframe on; spacefill off""
MarvinView: "navmode=zoom"
ViewerActiveX:"Mouse=4 Convert2Dto3D=0"
```

Try overriding default values or specify additional valid parameter/value pairs to get desired results. Example for using CPK rendering scheme with Jmol viewer:

```
"script="select *; set frank off; wireframe off; spacefill on""
```

--strviewerembed *direct* | *javascript*

Specify how to embed structure viewers in HTML pages. Possible values: *direct* - use applet/object tags to emded structure viewer; *javascript* - use vendor supplied java scripts. Default value: direct.

This option only applies to these vieweres: *Chem3DActiveX, ChemDrawActiveX, ChemDrawPlugIn, Jmol, and MarvinView*.

For marvin.js to work correctly on your browser, you may need to set *marvin_jvm=builtin* or *marvin_jvm=plugin* using --strviewerparams option. Additionally, MarvinView - at least in my hands - also has problems during usage of JavaScript for local deployment; however, it does work via web server.

As far as I can tell, Jmol.js supplied with Jmol10 release has these issues: jmolSetAppletColor doesn't support background color; jmolInitialize disables relative specification of codebase directroy which works okay. So, use Jmol.js supplied with MayaChemTools.

--strviewerjsfile *java script file name*

Name of vendor supplied java script file. Default values: Chem3DActiveX: *chem3d.js*; ChemDrawActiveX, and ChemDrawPlugIn: *chemdraw.js*; Jmol: *Jmol.js*, MarvinView: *marvin.js*.

Directory location for these files is specified via *codebase* value of --strviewerconfig option.

--strtablesize *"numrows,numcols"*

This option is only valid for *structuresonly* and *shadedstructuresonly* modes. And it indicates maximum number of rows and columns per structure table. Default value:*6,4*.

--stylesheet *old* | *new* | *none*

Controls usage of stylesheet for newly generated HTML file(s). Possible values: *old, new, or none*. Default value: *new*.

Stylesheet file contains various properties which control appearance of HTML pages: type, size, and color of fonts; background color; and so on.

For *old* value, an existing stylesheet file specified by --stylesheetname option is used for each HTML file; no new stylesheet file is created. This option is quite handy for deploying HTML file(s) on a web server: assuming you specify a valid stylesheet file location relative to your WWWRoot, a reference to this stylesheet is added to each HTML file. For local deployment of HTML file(s), a complete path to a local stylesheet is fine as well.

For *create* value, a new stylesheet is created and reference to this local stylesheet is added to each HTML file. Use option --stylesheetname to specify name.

For *none* value, stylesheet usage is completely ignored.

--stylesheetname *filename*

Stylesheet file name to be used in conjunction with -s --stylesheet option. It is only valid for *old* value of -s --stylesheet option. Specify a valid stylesheet file location relative to your WWWRoot and a reference to this stylesheet is added to each HTML file. Example: *"/stylesheets/MyStyleSheet.css"*. Or a complete path name to a local stylesheet file.

For *create* value of -s --stylesheet option, a new stylesheet file is created using -r --root option. And value of --stylesheetname is simply ignored.

--shadecolor *"#RRGGBB,#RRGGBB"*

Colors used to fill background of rows during *shade* and *shadedhightlight* mode represented as a pair of hexadecimal string; the first and second color values are used for odd and even number rows respectively.

Default value: *"#ffffff,#e0e9eb"* - it's white and very light blue for odd and even number rows.

-t, --title *string*

Title for HTML table(s). Default value: *SDFileName*. This option is ignored for multiple input files. And -r --root option is used to generate appropriate titles.

--titledisplay *yes* | *no*

Display title for HTML table(s). Possible values: *yes or no*. Default value: *yes*.

-w, --workingdir *dirname*

Location of working directory. Default: current directory.

EXAMPLES

HTML table file(s), containing structures, can be used in two different ways: browsing on a local machine or deployment via a web server. By default, HTML file(s) are created for viewing on a local machine using Jmol viewer through a browser; however, you can specify any supported applet viewer and generate HTML file(s) for deploying on a web server.

First two sets of examples show generation of HTML file(s) using different applet viewers and a variety of options for local browsing; last set deals with web deployment.

Local deployment: Usage of default JMol viewer distributed with MayaChemTools:

To generate HTML tables with structure display using JMol viewer, rows background filled with white and light blue colors, navigation links on top and botton of each page, type:

```
% SDFilesToHTML.pl -o Sample1.sdf
```

To generate HTML tables with structure display using JMol viewer, rows background filled with white and light blue colors, navigation links on top and botton of each page, and only containing MolWeight and Mol_ID SD data fields, type:

```
% SDFilesToHTML.pl --datafields "MolWeight,Mol_ID" -o Sample1.sdf
```

To generate HTML tables with CPK structure display using JMol viewer, rows background filled with white and light blue colors, navigation links on top and botton of each page, type:

```
% SDFilesToHTML.pl --strviewerparams "script=\"select *; set frank off;
  wireframe off; spacefill on\"" -o Sample1.sdf
```

To generate HTML tables with structure display using JMol viewer and black background, rows background filled with light golden and greyish colors, navigation links on top and botton of each page, 10 rows in each table, greyish header row color, and cell spacing of 1, type:

```
% SDFilesToHTML.pl -o -n 10 --headeralign "center" --headercolor
  "#a1a1a1" --shadecolor "#fafad2,#d1d1d1" --cellspacing 1
  --strviewerparams "bgcolor=#000000" Sample1.sdf
```

To highlight molecular weight values using specified highlight criteria and fill in default background colors, type:

```
% SDFilesToHTML.pl -n 10 --highlight "MolWeight,numeric,le,450"
  --highlightstyle background -m shadedhighlight -o Sample1.sdf
```

To highlight molecular weight values using specified highlight criteria, color the text using default colors, and add a footer message in every page, type:

```
% SDFilesToHTML.pl -n 4 --highlight "MolWeight,numeric,le,500"
  --highlightstyle text -m shadedhighlight -o
  --footer "Copyright (C) MayaChemTools" --cellspacing 1 Sample1.sdf
```

To generate tables containing only structures, type:

```
% SDFilesToHTML.pl -d both -m shadedstructuresonly --strtablesize "6,4"
  --cellspacing 1 -b 1 -o Sample1.sdf
```

To generate tables containing only structures with molecular weight displayed above the structure, type:

```
% SDFilesToHTML.pl -d both -m shadedstructuresonly --strtablesize "6,4"
  --cmpddatafield "MolWeight,no,top,center"  --cellspacing 1 -b 1
  -o Sample1.sdf
```

To generate tables containing links to structures and highlight molecular weight data field values using specified highlight criteria , type:

```
% SDFilesToHTML.pl -n 4 --footer "Copyright (C) MayaChemTools"
  --highlight "MolWeight,numeric,le,450" --highlightstyle background
  -d both -m shadedhighlight  -s link --strlinktype button
  -o Sample1.sdf
```

Local deployment: Usage of other structure viewers:

```
% SDFilesToHTML.pl --strviewertype MarvinView --strviewerconfig
  "<Marvin dir path>" -o Sample1.sdf
```

```
% SDFilesToHTML.pl -o -n 10 --headeralign "center" --headercolor
  "#a1a1a1" --shadecolor "#fafad2,#d1d1d1" --cellspacing 1
  --strviewerparams "bgcolor=#000000" --strviewertype Chime
  Sample1.sdf
```

```
% SDFilesToHTML.pl -n 10 --highlight "MolWeight,numeric,le,450"
  --highlightstyle background -m shadedhighlight --strviewertype
  Chime -o Sample1.sdf
```

```
% SDFilesToHTML.pl -d both -m shadedstructuresonly --strtablesize "6,4"
  --cellspacing 1 -b 1 -strviewertype JME -strviewerconfig "<JME dir
  path>" -o Sample1.sdf
```

Web deployment: Usage of different structure viewers and options:

For deploying HTML file(s) on a web server, specify a valid *codebase* directory name relative to <WWWRootDir>. In addition to *codebase*, you can also specify *archive* file name.

```
% SDFilesToHTML.pl -m plain -s display --strviewertype Jmol
  -strviewerconfig "/jmol" -n 5 -d both -r PlainTable -t "Example
  using Jmol: Plain Table" -o Sample1.sdf
```

```
% SDFilesToHTML.pl -n 5 -m shade  -s display -strviewertype JME
  -strviewerconfig "/jme,JME.jar" -r ShadeTable -t "Example using JME:
  Shaded Table" -o Sample.sdf
```

```
% SDFilesToHTML.pl -n 5 --highlight "MolWeight,numeric,le,450"
  --highlightstyle background  -d both -m shadedhighlight  -s display
  -strviewertype MarvinView -strviewerconfig "/marvin" -r
  ShadedHightlightTable -t "Example using MarvinView: Shaded and
  Highlighted Table" -o Sample.sdf
```

```
% SDFilesToHTML.pl -n 4 --highlight "MolWeight,numeric,le,450" -s link
  --strlinktype href --strviewertype ChemDrawPlugIn  --highlightstyle
  background -m shadedhighlight -t "Example using ChemDrawPlugIn:
  Shaded and Highlighted Table" -r ShadedHightlightTable -o Sample1.sdf
```

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

FilterSDFiles.pl, InfoSDFiles.pl, SplitSDFiles.pl, MergeTextFilesWithSD.pl

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