
INSTALLING THE XEMISTRY WEB SKETCHER ON MS WINDOWS SYSTEMS RUNNING THE IIS WEB SERVER

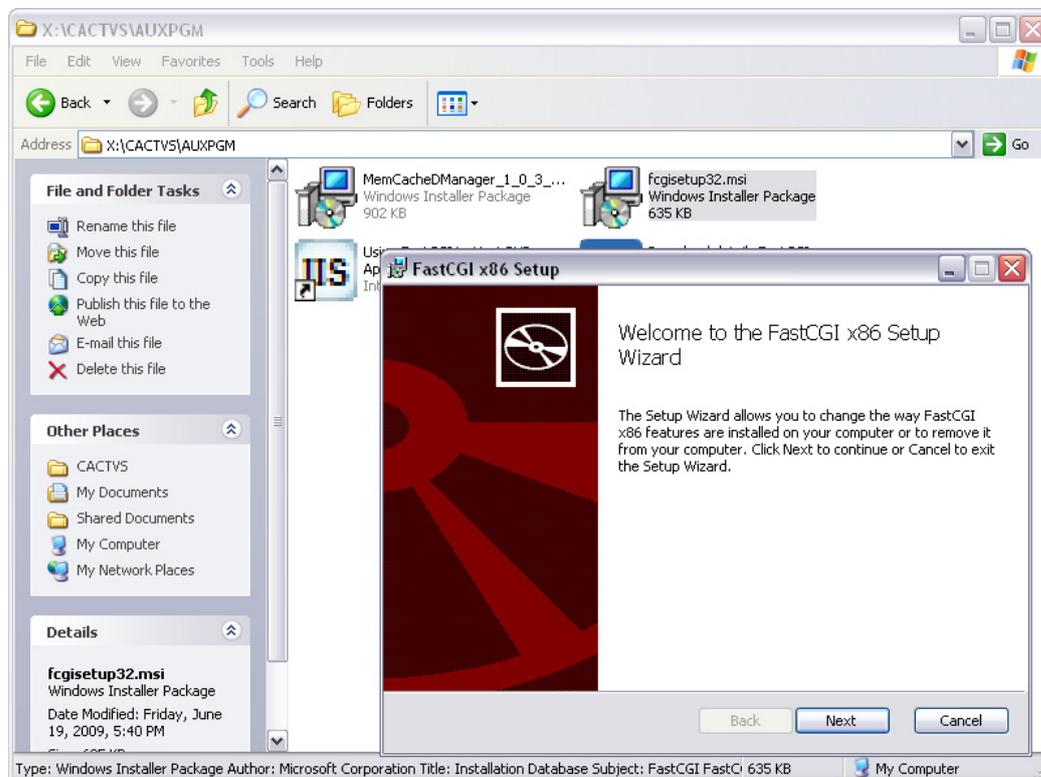
This is a step-by-step introduction to set up the Web sketcher application on a Windows server. This manual assumes that you are familiar with basic Windows administration, and that you have sufficient permissions to install executables, administer the IIS settings, and create new Websites.

STEP 1: VERIFY THAT YOU HAVE A WORKING WEB SERVER ON YOUR SYSTEM

IIS is not installed by default on all Windows versions. Make sure that your server has a properly configured and running IIS (Internet Information Server, the default Web server for Windows systems), and that you can load Web pages and active content from other sites on the installation system using a standard browser such as Internet Explorer. Also, it is a good idea to locate the server logs (usually in a place like C:\windows\system32\logfiles\W3SVC1) so that you know where to check in case something does not work as expected.

STEP 2: INSTALL THE FCGI MODULE

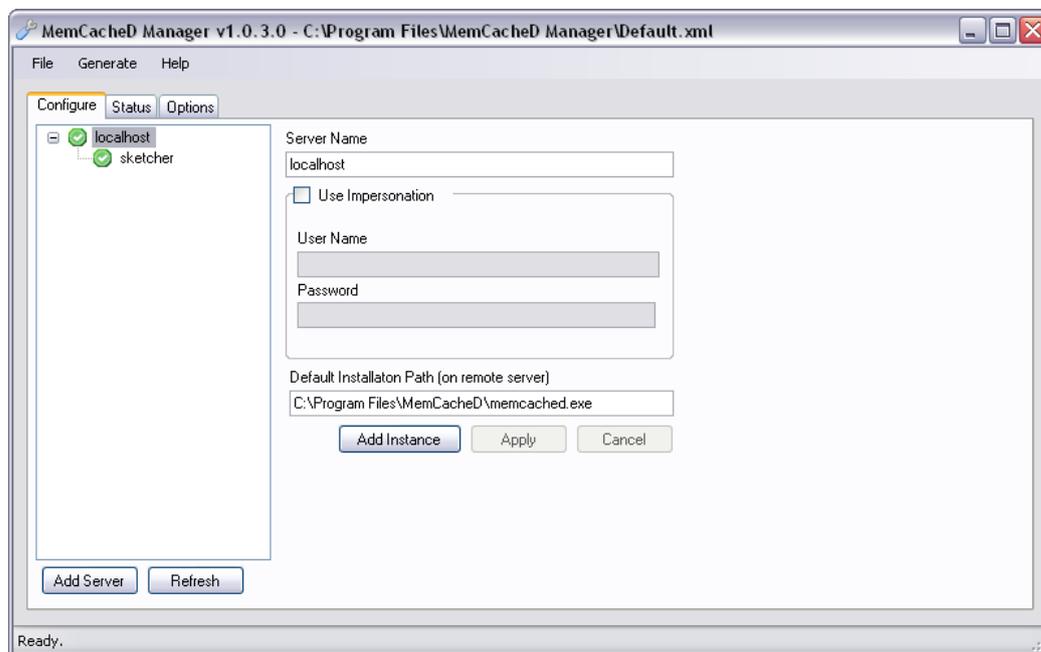
Download the fcgisetup32.msi installable, if you Web server does not already run FCGI applications. Perform a normal installation procedure with this package. Further information on this application can be found at <http://forums.iis.net/1103.aspx>. Locate the place the FCGI DLL is stored (usually C:\WINDOWS\system32\inetsrv\fcgiext.dll) and jot it down.



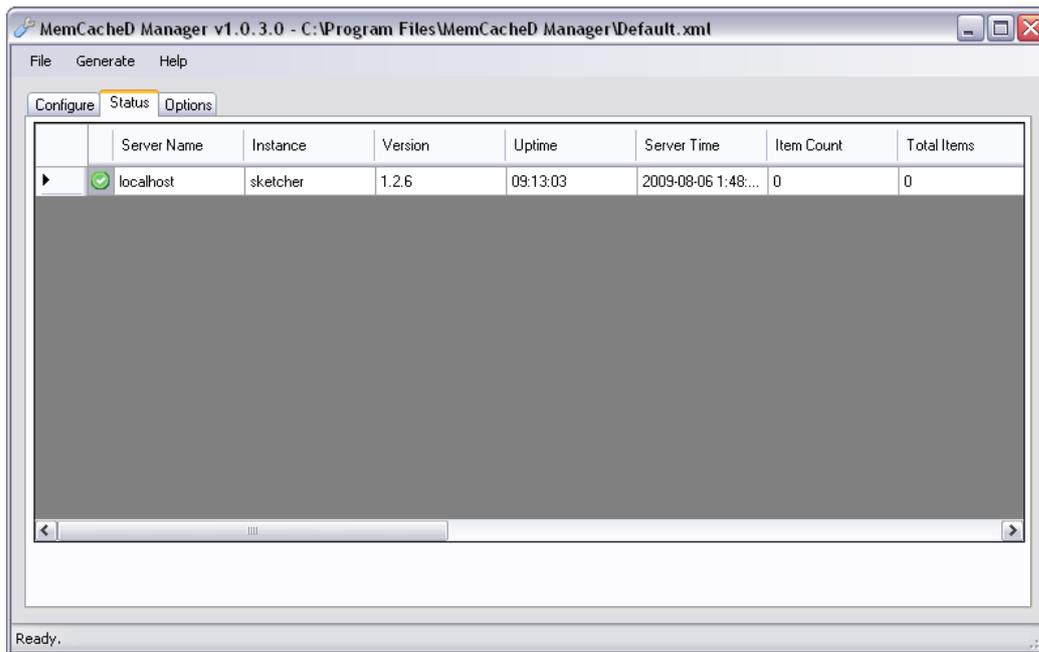
STEP 3: INSTALL THE MEMCACHED SERVICE

Next, download the MemCacheDManager_1_0_3_0.msi installation package and run it, if your system does not already support the memcached service. Memcached is used to store the state of the sketcher (i.e. the current and backup structures with all layout information). The cache daemon does not necessarily need to run on the same system as the main sketcher application. In case there are multiple sketcher hosts with some kind of dynamic load balancing system, it is mandatory that the cache daemon is only run on a single system and all sketcher hosts are pointed to a common storage host later in the installation. Nevertheless, for all but the most heavily frequented sites a single sketcher FCGI instance with the caching daemon running on the same host will be sufficient. A sketcher instance can support dozens of simultaneous clients without generating noticeable loads on reasonably powerful servers.

After installation, run the newly installed Memcached Manager application and set up one service instance (called *sketcher* in the screenshot, but the name does not really matter). The default parameters are fine. Do not change the port setting or IP address parameters except you really know what you are doing, and are prepared to perform some tricky adjustments in other parts of the system. The caching daemon instance configured with the aid of this tool is automatically set up to operate as a standard Windows service. It is automatically restarted when the computer is rebooted.



Make sure that the service is now running by checking the status tab.



STEP 3: GET INSTALLATION SUPPORT TOOLS

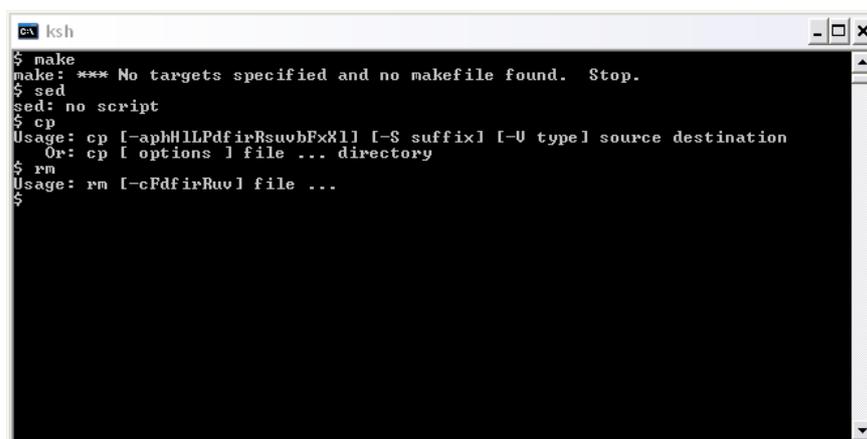
The Web sketcher was originally developed as a Linux/Apache application, and is therefore most conveniently installed in a Unix-style fashion with the aid of an installation Makefile. This Makefile requires the presence of a couple of standard Unix tools.

Fortunately, it is not complicated to install a compatible tool set on a Windows system thanks to the people at AT&T and their U/WIN package.

Download the U/WIN base and dev packages. You do not need the additional X-windows, fonts and other auxiliary packages. Run the installation, and open the ksh (Korn shell) window by clicking on the



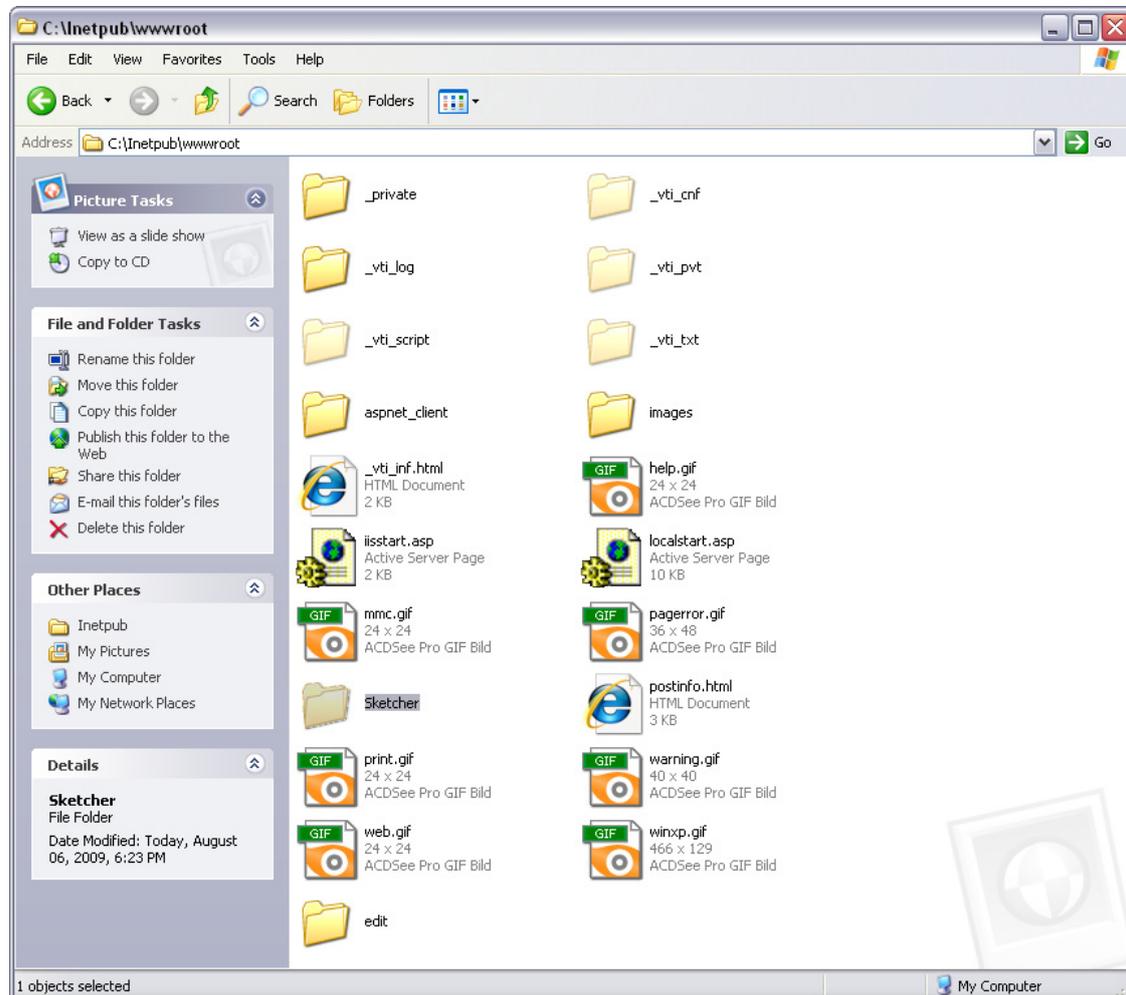
desktop icon. The opened application window looks much like a simple Windows command window, but provides access to a much richer and Linux/Unix compatible command set. Make sure that the required tools, such as Unix-style make, the *sed* stream editor, *cp*, *rm* and other basic tools are accessible.



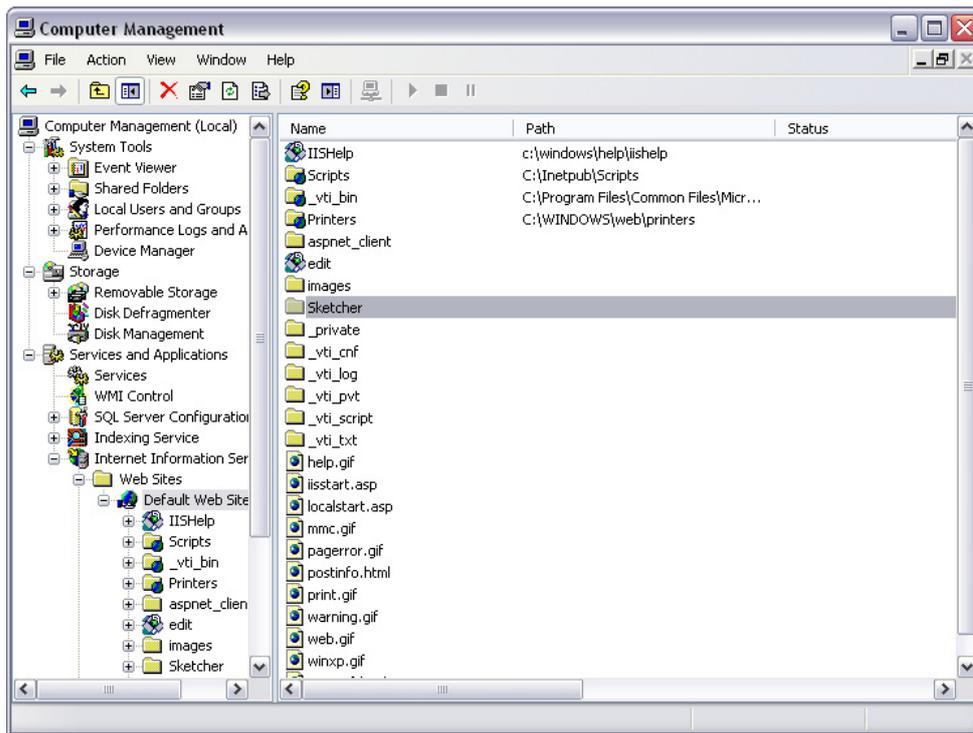
The error messages in the screenshot are nothing to worry about. This just checks that the required tools are found. The U/WIN tools are only needed for installation, not for server operation. They can be uninstalled once the system has been set up if desired.

STEP 4: CONFIGURE A NEW WEBSITE IN IIS

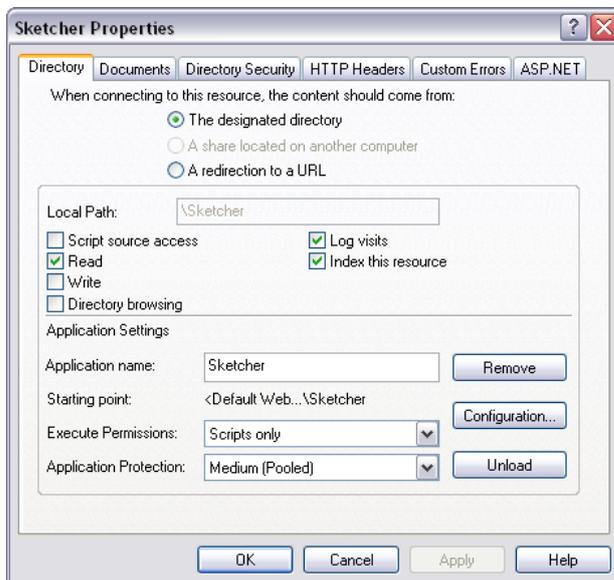
First, use the normal file browser to set up a normal file system directory for the sketcher (named *Sketcher* in this example). This is not the same as setting up a virtual directory in the computer management tool – you will need to use the file explorer!



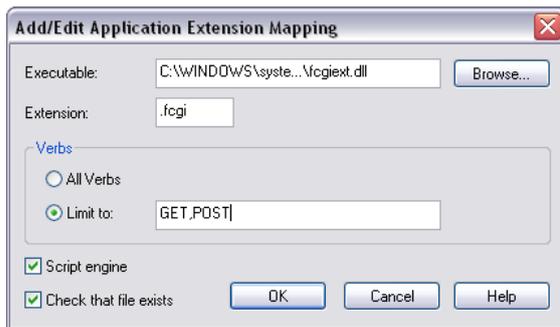
Next, start the computer management console and open the item tree until you find the IIS Default Web Site item, with our new directory embedded in it.



Right click on it and open the properties panel. Create a new application for this directory by clicking on the button next to the *Application Name* line, and then enter an application name - here it is also named *Sketcher*.



Next, click on the Configuration button and add an extension mapping for the suffix .fcgi to the IIS CGI extension DLL whose address you remembered in an earlier installation step. This extension needs to be marked as a script engine, and be activated for the GET and POST methods, as shown below.



Because of a documented bug found at least in the Win XP version of this tool, the OK button on this panel, after loading the DLL path from the file selector, will only become active by clicking into the *Executable* text line with the mouse pointer once more, without changing anything.

STEP 5: CONFIGURE THE FCGI IIS MODULE

Use the file explorer to locate the file *fcgiext.ini* in the same directory as the IIS FCGI module DLL and open it in a text editor. Change the configuration section to

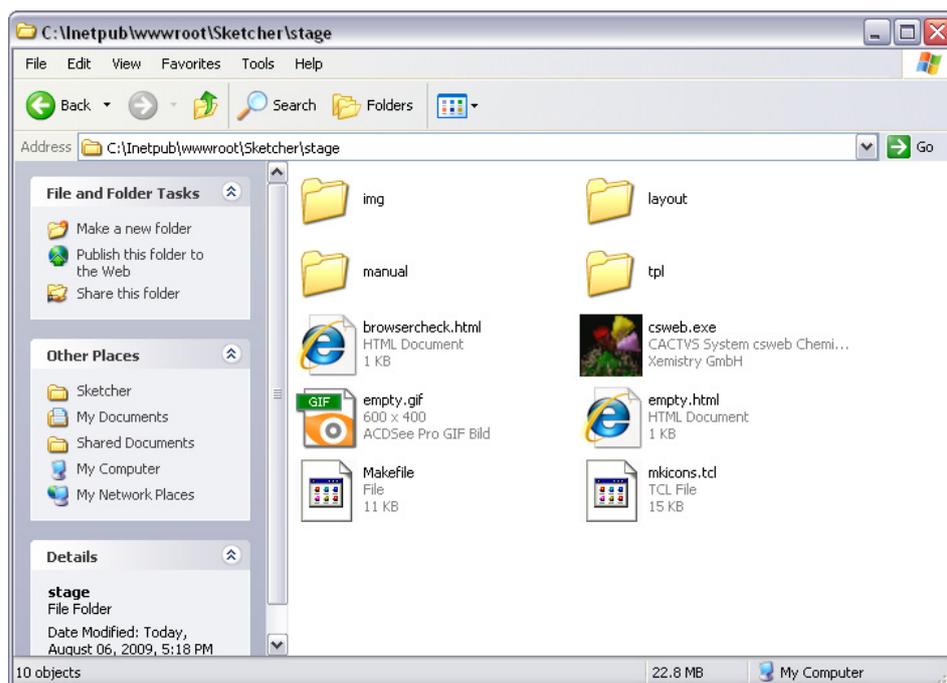
```
[Types]
fcgi=Sketcher
[Sketcher]
ExePath=C:\inetpub\wwwroot\INSTALLDIR\csweb.exe
Arguments=-f C:\inetpub\wwwroot\INSTALLDIR\editsrv.fcgi
ActivityTimeout=10
InstanceMaxRequests=10000
StderrMode=IgnoreAndReturn200
MonitorChangesTo=C:\inetpub\wwwroot\INSTALLDIR\editsrv.fcgi
```

where the *INSTALLDIR* part is changed to the name of the directory was just created in the previous step, and the path to the root Web directory is also adjusted, if required. There is a required space between *-f* and the rest of the line for the *Arguments* parameter, which is important. Save the file in place. Then, restart IIS from the Computer Management Console and watch for any reports of syntax errors in the configuration file.

In case the FCGI module serves additional applications, add the Sketcher section as an additional entry in proper fashion instead of replacing everything.

STEP 6: EXPAND THE SKETCHER SOURCE PACKAGE.

Get the zip package with the sketcher application files and expand it in the newly configured disk directory for the sketcher Web application. You will see a single new directory called *stage*, which contains all software and templates needed for the sketcher application proper.



First, let us verify some basic functions. Open the ksh window, navigate into the sketcher installation directory and then further into the staging directory, and execute a couple of commands:

```

C:\ ksh
$ cd C:/inetpub/wwwroot/Sketcher/stage
$ ./csweb -v
csweb U3.360
Developer: Xemistry GmbH
Distributor: Xemistry GmbH
Licensee: ChemSpider
License Type: Commercial
$ ./csweb
cactus>memcache create localhost
memcache0
cactus>memcache put memcache0 testkey testdata
testkey
cactus>memcache get memcache0 testkey
testdata
cactus>memcache status memcache0
pid 1116 uptime 46035 time 1249572161 version 1.2.6 cmd_flush 0 accepting_conns
0 listen_disabled_num 0 bytes_read 36823 bytes_written 1137537 curr_connections
12 total_connections 18 get_hits 15 get_misses 0 curr_items 9 total_items 21 thr
eads 1
cactus>exit
$

```

The first command verifies that the script interpreter works. The second set of commands in the interactive interpreter checks interaction with the memcached service. The exact results for the service status query may be different, but there should be no errors or time-outs.

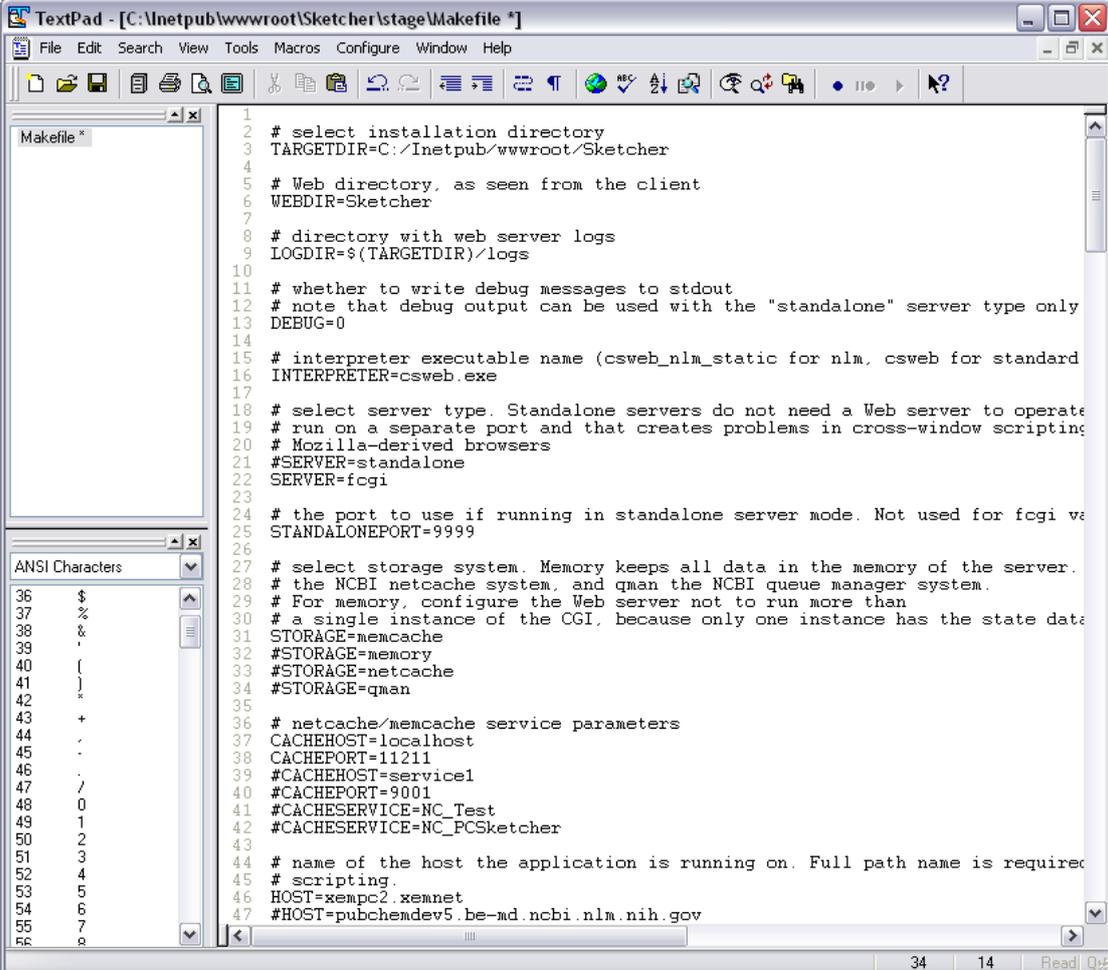
STEP 7: CONFIGURING THE SKETCHER INSTALLATION

In the staging directory, there is a file called Makefile. Open it in a plain text editor like *notepad* or *textpad* (not MS Word!) and configure the Makefile variables in the first lines according to your set-up. The most important three items are:

TARGETDIR: The full path of the installation directory, directly below the stage directory. Use forward slashes, not backslashes for directory separation.

WEBDIR: The path to the installation directory from the Web root, as seen from a Web browser. Do not use a leading slash.

HOST: The full domain-resolved name of the server. The domain part is important if you want to support data exchange with Web forms which are hosted in the same fundamental domain, but not the same subdomain. If this is not configured correctly, data exchange via JavaScript functions may be seen as cross-site scripting security violation and suppressed by the Web browser, resulting in the inability to transfer data between a recipient application form and the sketcher.



```
1 # select installation directory
2 TARGETDIR=C:\inetpub\wwwroot\Sketcher
3
4
5 # Web directory, as seen from the client
6 WEBDIR=Sketcher
7
8 # directory with web server logs
9 LOGDIR=$(TARGETDIR)/logs
10
11 # whether to write debug messages to stdout
12 # note that debug output can be used with the "standalone" server type only
13 DEBUG=0
14
15 # interpreter executable name (csweb_nlm_static for nlm, csweb for standard
16 INTERPRETER=csweb.exe
17
18 # select server type. Standalone servers do not need a Web server to operate
19 # run on a separate port and that creates problems in cross-window scripting
20 # Mozilla-derived browsers
21 #SERVER=standalone
22 SERVER=fcgi
23
24 # the port to use if running in standalone server mode. Not used for fcgi ve
25 STANDALONEPORT=9999
26
27 # select storage system. Memory keeps all data in the memory of the server.
28 # the NCBI netcache system, and qman the NCBI queue manager system.
29 # For memory, configure the Web server not to run more than
30 # a single instance of the CGI, because only one instance has the state data
31 STORAGE=memcache
32 #STORAGE=memory
33 #STORAGE=netcache
34 #STORAGE=qman
35
36 # netcache/memcache service parameters
37 CACHEHOST=localhost
38 CACHEPORT=11211
39 #CACHEHOST=service1
40 #CACHEPORT=9001
41 #CACHESERVICE=NC_Test
42 #CACHESERVICE=NC_PCSketcher
43
44 # name of the host the application is running on. Full path name is required
45 # scripting.
46 HOST=xempc2.xemnet
47 #HOST=pubchemdev5.be-md.ncbi.nlm.nih.gov
```

It is recommended not to change the LOGDIR, DEBUG, INTERPRETER, STORAGE or SERVER variables. Most of these are only meaningful for Linux installations. The Windows version only supports the FCGI application style in connection with a memcached state store service. Also, logging and debugging require that you can forward standard error channel data from the FCGI application to the Web server log file, which is not supported by the Windows FCGI IIS module.

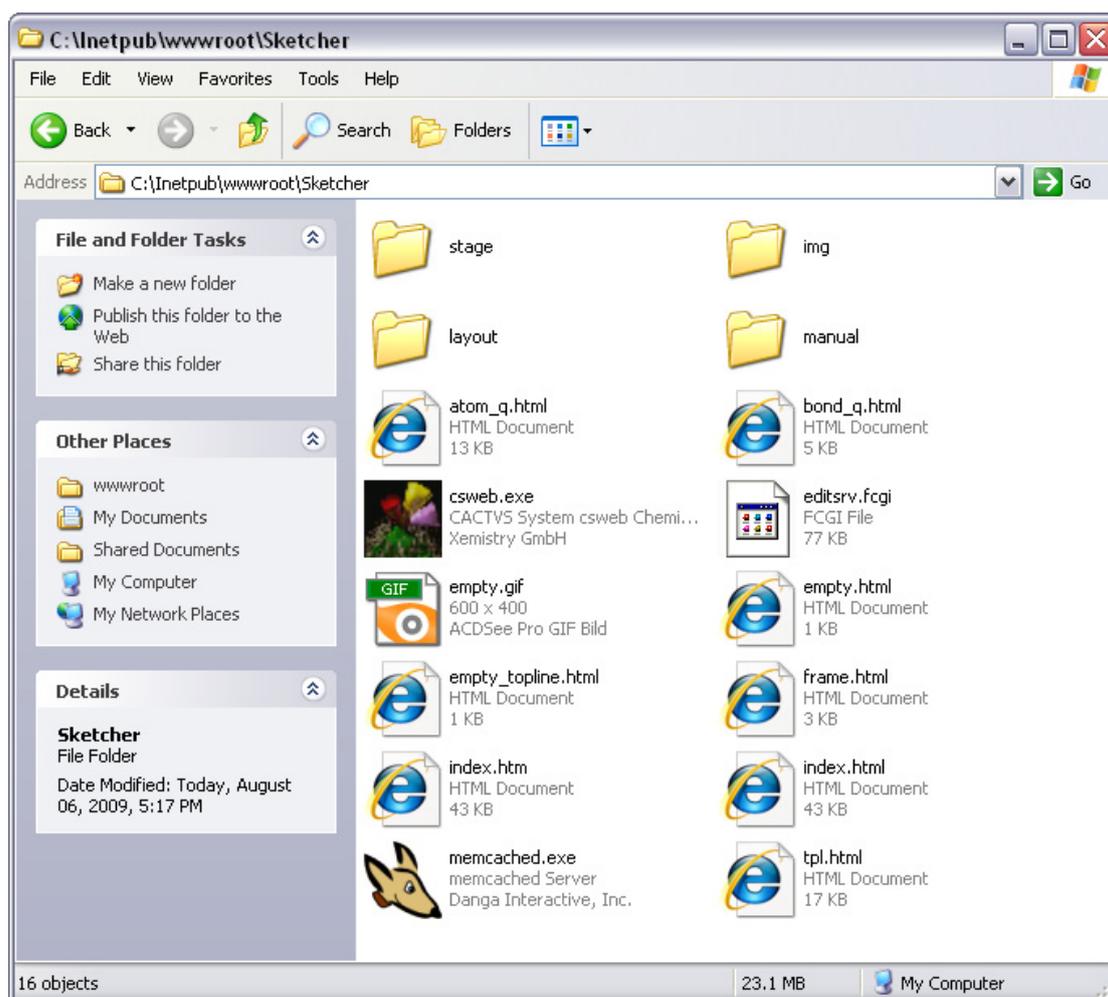
If this has all been configured correctly, store the edited Makefile in place and enter the ksh command window again. Make sure the current directory is the staging directory. There, type *make* and hit return once, thereby answering the question whether you want to regenerate the interface icons with a negative.

```

c:\ ksh
cp `which csweb.exe` C:/Inetpub/wwwroot/Sketcher; \
fi
chmod +x C:/Inetpub/wwwroot/Sketcher/csweb.exe
chmod +x C:/Inetpub/wwwroot/Sketcher/editsrv
if [ "fcgi" = "fcgi" ]; then \
  mv C:/Inetpub/wwwroot/Sketcher/editsrv C:/Inetpub/wwwroot/Sketcher/edit
srv.fcgi; \
  chmod +x C:/Inetpub/wwwroot/Sketcher/editsrv.fcgi; \
else \
  rm -f C:/Inetpub/wwwroot/Sketcher/editsrv.fcgi; \
fi
if [ "memcached" = "memcached" ]; then \
  rm -f C:/Inetpub/wwwroot/Sketcher/memcached; \
  if [ -x ./memcached ]; then \
    cp memcached C:/Inetpub/wwwroot/Sketcher; \
  else \
    cp `which memcached` C:/Inetpub/wwwroot/Sketcher; \
  fi; \
  chmod +x C:/Inetpub/wwwroot/Sketcher/memcached; \
fi
cp -r manual/HTML/Sketcher\ Manual/Output/* C:/Inetpub/wwwroot/Sketcher/manual
mv C:/Inetpub/wwwroot/Sketcher/manual/Frameset.html C:/Inetpub/wwwroot/Sketcher
/manual/index.html
rm -f C:/Inetpub/wwwroot/Sketcher/Makefile
$

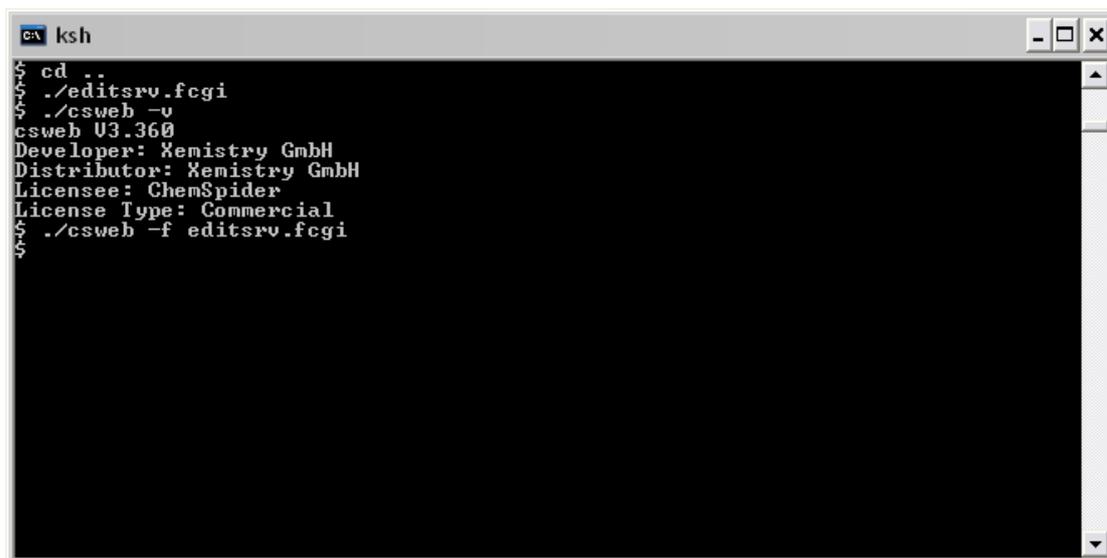
```

If all goes right, a few lines of printouts of commands will scroll by, and the directory one level upwards – the base installation directory - is populated with files patched with the values of the Makefile variables.



The file explorer window above shows the contents of the Sketcher base installation directory after running the installation script.

Go one directory level upwards in the ksh command window, and verify that the configured FCGI script can be executed:



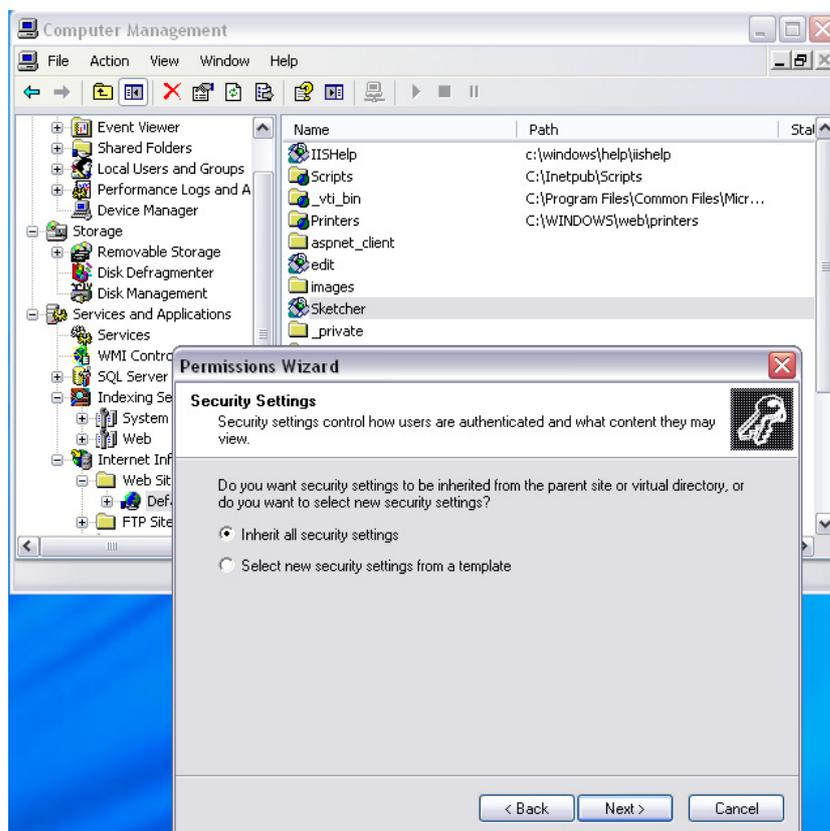
```

c:\ ksh
$ cd ..
$ ./editsrv.fcgi
$ ./csweb -v
csweb U3.360
Developer: Xemistry GmbH
Distributor: Xemistry GmbH
Licensee: ChemSpider
License Type: Commercial
$ ./csweb -f editsrv.fcgi
$

```

There should be no error messages.

The final step is to make sure the permissions of all the files are set correctly. Go back to the computer management console, right-click on the Sketcher directory, and run the permissions wizard.



The default options “Inherit all security settings” and, on the next panel, “Replace all directory and file permissions” are correct choices.

