

File and directory structure of GPMaw

Default installation

Upon installation of the current version 10 the following files are installed:

\gpmaw

Setup.log – file created by the install program for the automatic de-installation of the program.

\gpmaw\bin

Gpmaw3.exe – main program

Gpmaw.lcs, **gpmaw.chk** – license files, only the .lcs file is needed, the .chk file may be removed.

Gpmaw.ini – default parameters of gpmaw.

Gpmaw.chm – help file

Formatdb.exe, blastall.exe – NCBI blast program, called from gpmaw

DbIndex.exe, dbindex.hlp – program for indexing databases. Run independently or called from gpmaw.

Fragment.exe – program for the de novo analysis of ms/ms spectra. Run independently or called from gpmaw.

Gdiplus.dll – a Windows dll missing from older version of Windows (to be removed in future installs)

PeakErazor.exe, keratin.lst – a program for removing contaminants from ms peak lists. Independent or called from gpmaw.

\gpmaw\bin\XTandem

Tandem.exe – program til søgning af ms/ms data mod en sekvens eller database

Input.xml, default_input.xml, taxonomy.xml – files updated by gpmaw for each search

Fasta_pro.exe – program for generating compacted searchable fasta formatted files

Readme.txt, license.txt – license of X!Tandem

Tandem-style.xsl, tandem-style.css, tandem-input-style.xsl – files used by tandem.exe

\gpmaw\bin\ClustalW

clustalw.exe – program til multiple alignments of sequences

clustal-help.txt – associated help file.

\gpmaw\bin\DATA\ or \gpmaw\bin

Blosum45, blosum62, blosum80, pam30, pam70, seqcode.val – matrix files used by the blastp program

\gpmaw\bin\documents

Document files in pdf format, mainly the Dummies guide and the full manual.

\gpmaw\system

***.mss** – mass files used by gpmaw for determining amino acid mass values. aa_mass.mss is the default mass file and essential for running the program.

***.mod** – modification files. Contains information on amino acid modifications.

Terminals.tms – list of mass values for the N- and C-terminals, including modifications.

Unimod.xml – list of chemical modifications of amino acids (originates from unimod.org).

\gpmaw\user

Blood.seq, insulin.seq – protein sequence files. Examples for the user to start out with.

Essential files for running gpmaw

A minimum system for running gpmaw can be created by only including the files listed in red in the above table. If the ini file is missing, gpmaw will throw up a number of warnings, but generate a new ini-file with default values. In this case you should open the System|Setup system dialog and review all settings, in particular directories for system and user files.

Files modified by the user/gpmaw

These files/directories need to have write access, see also Windows UAC below.

Gpmaw.ini – contains all user settings and atom mass values. By default stored in base directory (\gpmaw\bin\).

User directory – Contains user-defined sequence files etc. Default is \gpmaw\user\. The directory can be changed in the System Setup to anywhere on the computer or network.

System directory – Contains general files (e.g. mass files) used by gpmaw. Default is \gpmaw\user\. The directory can be changed in the System Setup to anywhere on the computer or network.

XTandem directory – X!Tandem is an external ms/ms search engine (www.thegpm.org). Default directory is \gpmaw\bin\xtandem\. As the control of the search program takes place through xml files written to this directory, the user needs access. This situation will be changed from version 9.10, where the user directory will be used.

Gpmaw and Windows User Access Control (UAC)

With the introduction of Vista, Microsoft also introduced User Access Control, which means that the user without administrator rights does not have access to the Program Files folder, Windows or System32 etc. This means that the standard setup of fails as gpmaw is not able to update its .ini file. In addition, some of the external programs, in particular X!Tandem, as communication between gpmaw and the external

program communicates takes place through files written to disk. In version 9 you can change the way gpmaw saves its files, from the gpmaw directory to the user directory. Due to compatibility with previous versions, you can set a number of options (in Setup|Setup system|Directories – Change file admin):

- Option 1) Keep the directory layout as described at the top of this document. This will in most cases demand administrator rights on Win7 and Vista machines.
- Option 2) Each user data resides in the user profile, specifically in [user profile]\AppData\Roaming\gpmaw and in the system and user directories below.
- Option 3) Each user data resides in the public user profile, specifically the ini- and communication-files are in [public profile]\Documents\gpmaw\. The user files are in the user directory below. System files (e.g. .mss og .mod) are in \ProgramData\gpmaw\system\. All user-configurable data are thus shared among different users.
- Option 4) All user configurable data are stored in the local profile, eg ini file in [user profile]\Documents\gpmaw and user data in in [user profile]\Documents\gpmaw\user. System data (e.g. .mss og .mod) are in \ProgramData\gpmaw\system\. User-configurable data are thus mostly private, and only gpmaw system data are shared.

During startup, gpmaw checks for the location of the gpmaw.ini file, starting from option 4 going through to option 1 and starts up in the corresponding mode. If only option 1 is found and the user is not administrator, a dialog pops up asking to change directory mode.