

GPMAW

Protein sequence analysis – the easy way

For many years now the amount of nucleotide sequence data has increased exponentially. Along with the nucleotide sequences the protein sequence data has increased. You cannot any longer keep track of sequences with a couple of document in your favourite word processor, but you need a professional level sequence handling program to save and analyse protein primary structures. Although a number of bioinformatics programs are available from various companies, most of these are mainly targeted at nucleotide sequence analysis. If you are working with mass spectrometry, you are doubly hit, as several of these programs don't even know the difference between monoisotopic and average masses – an essential requirement with today's high-resolution instruments.

Product overview

GPMAW is designed to handle multiple protein sequences simultaneously. These may be imported from a number of sources. Based on the primary structure a large number of operations can be performed, and a number of physical/chemical properties calculated. In order to cater for the hugely increasing popularity of mass spectrometry, protein and peptide masses can be reported as monoisotopic or isotopically averaged, precision can be defined as 2 or 4 decimals, multiply charged species as well as positively and negatively charged molecules can be calculated.

Protein sequence import

Protein sequences may be entered manually in the built-in sequence editor, or they may be pasted from the clipboard in a number of sequence formats. FastA, EMBL (Swiss-Prot) and GenPept (NCBI, Entrez) formats are immediately recognised, while other text formats may be pasted into the "Import sequence" dialog which facilitates easy transfer of information to GPMAW. Local databases in FastA format may be indexed and accessed locally or across a LAN. The Entrez database can be searched directly across the net (may not work though a firewall).

Sequences can be saved in local files including all annotations (editable). If the sequence is imported from the Swiss-Prot database you will be able to import many of the secondary modifications listed in the annotation by the click of the mouse.

Sequence handling

Sequences up to a length of 8000 residues may be entered and defined as consisting of up to 7 polypeptides. Individual residues and/or groups of residues may be modified (i.e. having a different chemical composition and mass) and chemically cross-linked (most kinds of linkages can be constructed, including disulfide bonds). Based upon the primary structure, a number of chemical physical parameters are calculated (e.g. mass, absorption, hydrophobicity etc.). Visually the sequence may be represented in 1- or 3-letter code, numbered and colored in user-defined ways. Parts of the sequence may be highlighted in order to quickly analyse for correct mass or to subdivide the sequence into sub-sequences. Multiple sequences may be opened simultaneously.

System requirements

GPMAW is a 32-bit Windows program that runs on all 32-bit Windows platforms (e.g. Win9x, NT and 2000). An older version with limited functionality is available for Windows 3.1.

Minimum hardware

5 MB hard drive space (without databases), 166 MHz Pentium, 32 MB RAM. 200 MHz Pentium or faster recommended.

Demo version

A demo version of the program is available for download from <http://welcome.to/gpmaw/> You may also request the demo on CD-ROM from Lighthouse data (php@bmb.sdu.dk).

This is a fully functioning version that is limited only in that it can only run 15 times on the same computer, and it is version 4.04. Please note that not all functions mentioned in this note are available in the demo.

In the package

The software is delivered with a 220+ page printed manual, an introductory booklet with hints and tips, a CD-ROM containing the program and databases (actual content see below). Registered customers will be informed by e-mail of new upgrades, which are free for the first twelve month after purchase.

Support

Free technical support is supplied either by e-mail (php@bmb.sdu.dk) or by fax (+45 66 19 33 96).

Peptides

A central theme is the generation and handling of peptides. These may be easily generated from a protein sequence based on a flexible peptide generation scheme. Templates for the most typical enzymes and chemicals are supplied, and the users can easily generate additional templates.

Once generated the peptides are reported with masses, HPLC indices, charge, theoretical pI and a number of other parameters. The list can be sorted by any parameter, and the list exported to spreadsheet or documents.

Based on the peptide list, graphical HPLC retention maps, mass spectra and charge vs. pH curves can be generated.

Each peptide can be further analysed, either as sequence ladder or as ms/ms cleavage (generating a/b/c/x/y/z fragment ions).

Mass searches

Single proteins may be searched for masses from a mass list (entered manually or imported from various instruments/programs) taking user-defined modifications, contaminations and enzyme specificity into account. The results can be linked back to the original sequence to show coverage.

On the other hand, FastA formatted databases (user generated or public domain databases downloaded from the web) can be searched for a peptide mass map and the results imported into GPMaw for further analysis.

Mass spectral analysis of chemically cross-linked proteins (surface topology or protein interaction studies) is also supported.

Sequence analysis

Local sequence databases may be searched by the BLAST program (included) called directly from GPMaw.

Based on the protein sequence graphs for hydrophobicity, charge vs pH or secondary structure may be generated. Dot-plots for comparing the identity of proteins are available. As a more exotic example, 2D-gels of a complete FastA formatted database can be generated and compared to proteins in GPMaw. The proteins behaviour in a 2D-gel upon trimming of either terminal can be simulated.

Upgrading

In the world of science, methods and techniques develop at a pace that seems to be ever increasing.

In order for the users of GPMaw to take advantage of new features, the program is upgraded incrementally, with a new release approximately every three months.

The upgrades are **free** for twelve months after purchase and can be downloaded from the web site:

<http://welcome.to/gpmaw>.

Registered customers are informed by e-mail of new updates. Other interested parties may register for the information by contacting Lighthouse data.

On the CD-ROM

GPMaw is delivered on a CD-ROM containing the GPMaw program, a database indexing utility and two protein databases, Swiss-Prot* and EMBL non-redundant. The databases are indexed and ready to use for text search and sequence retrieval. They can be used for peptide mass searching after using the included derivatisation command.

*Please note that commercial users require a license from EBI to use the Swiss-Prot database

Pricing information (valid until July 1st 2002)

Full version of GPMaw v. 5.01..... US\$ 240.00
Additional copies

when ordered together (-25%) US\$ 180.00

Upgrades from previous versions are entitled to 50% discount on the above prices when old license number(s) are supplied.

The price is ex. VAT but includes postage and delivery. Local taxes and/or customs duty are not included. EU customers should supply a valid company SE number.

The invoice will be in local currency based on current exchange rates. If you need a quote or want a site license, please contact Lighthouse data on php@bmb.sdu.dk.

Payment is 30 days when using a purchase order. Please pay by check or bank transfer. Credit cards (Visa/Mastercard/Eurocard) are accepted; please contact Lighthouse data for an order form.

Ordering information

Please order your copy of GPMaw from

Lighthouse data

Engvej 35

DK-5230 Odense M

Denmark

Fax: (+45) 6619 3396

Mail: php@bmb.sdu.dk

When ordering please include:

- 1) Delivery address
- 2) Invoice address
- 3) Contact person (+ fax or e-mail number)
- 4) Purchase order number (if applicable)
- 5) VAT number if ordering from an EU country.

Web: <http://welcome.to/gpmaw>