



CometUI

User Guide

Comet UI Version 1.0.0.0

Comet Search Engine Version 2015.02 rev. 0

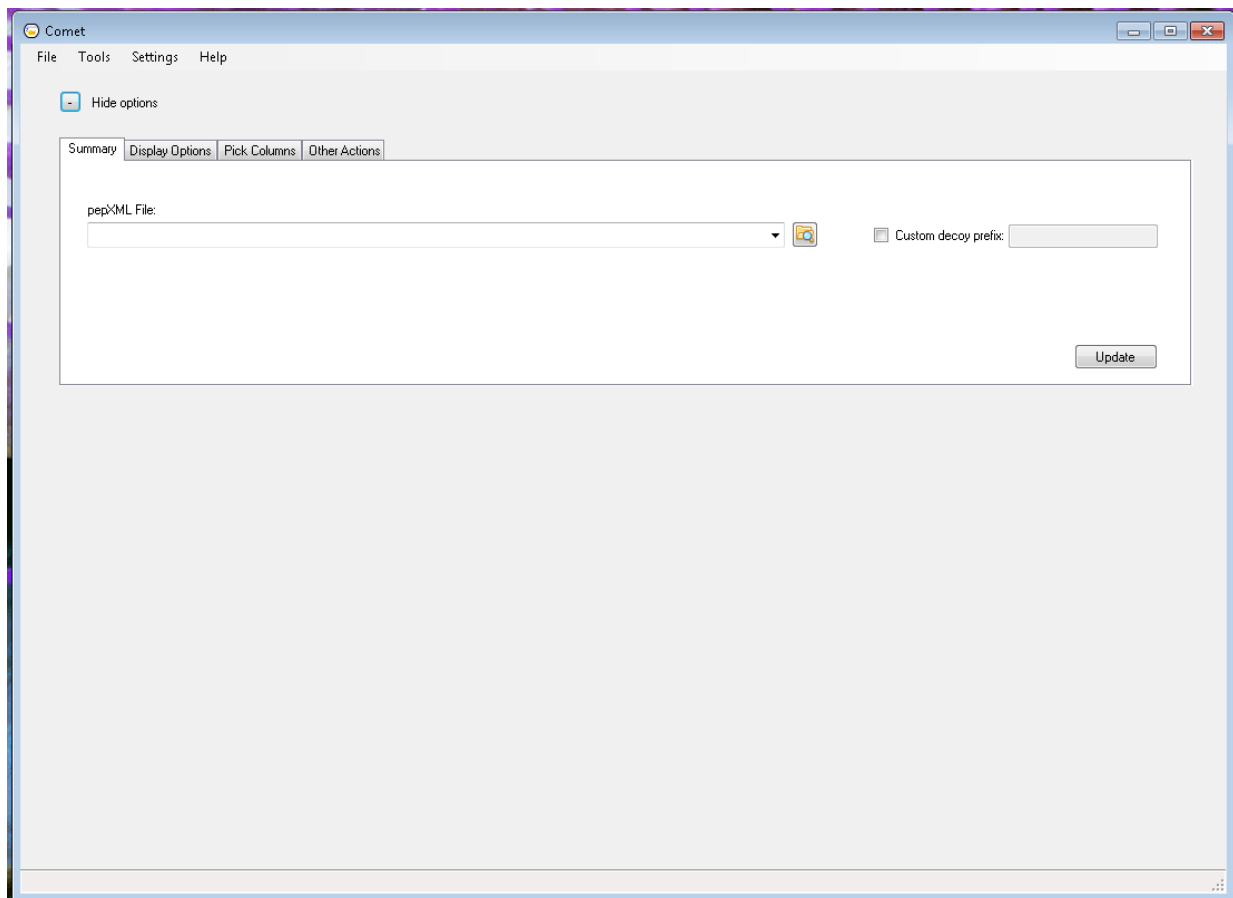
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Introduction

This document describes features of the CometUI application, a Windows-based graphical user interface used to run the Comet search engine and interrogate results. Users can also use CometUI to edit Comet search parameters, and import/export them from/to a “.params” file used by the command line version of the Comet search engine.

Users can download CometUI from the [Comet website](#). Launching the application will bring up the following window:



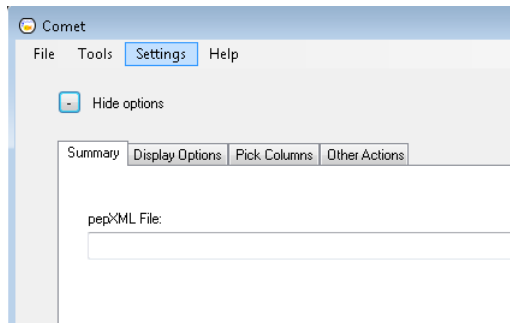
This document will describe how to navigate this window to perform the following tasks:

- View and Edit Search Settings
- Save Search Settings
- Import/Export Search Settings
- Run Search
- View Search Results

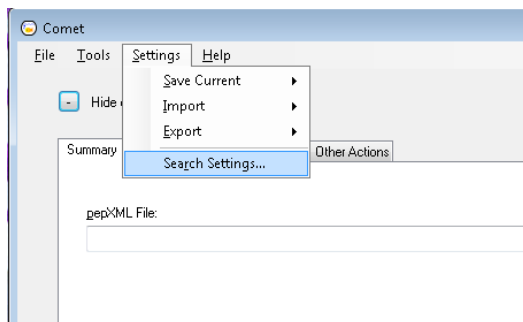
View and Edit Search Settings

All the search parameters and their default values in the Search Settings dialog correspond to [Comet search parameters](#) listed on the Comet website. To view/edit the search parameters, open the Search Settings dialog:

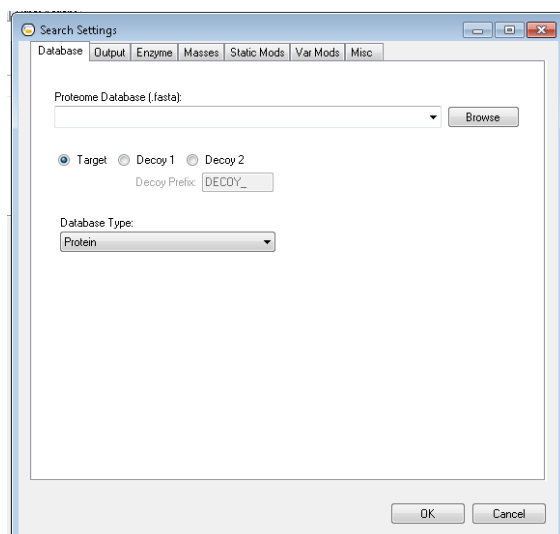
1. Click on the “**Settings**” menu:



2. Choose the “**Search Settings...**” menu item:

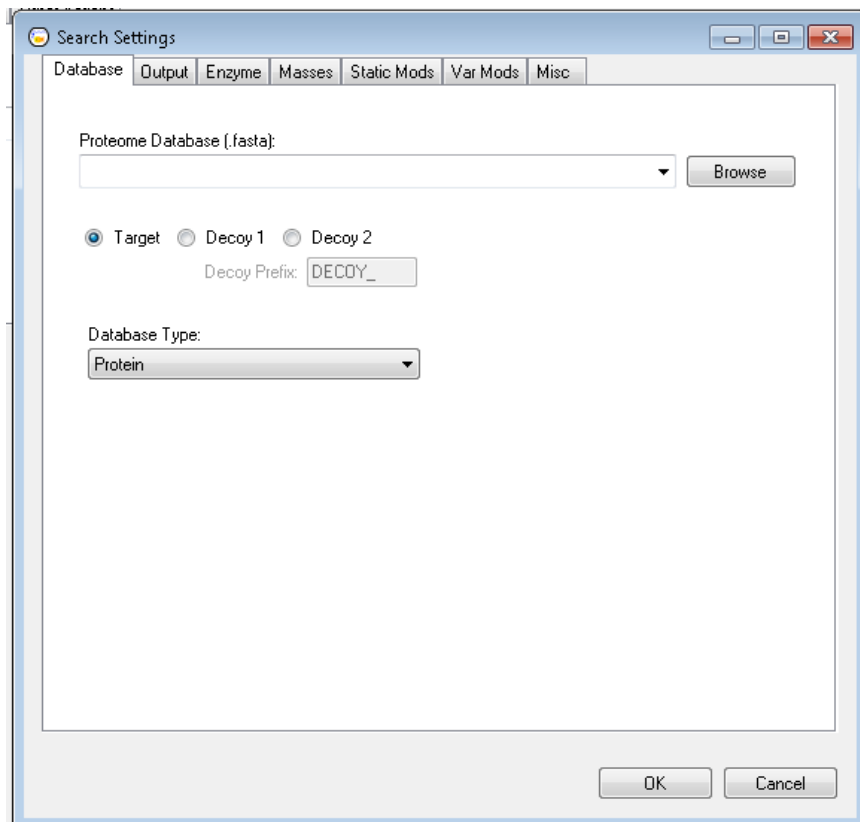


3. The following dialog should open up:



Database Search Settings Tab

The “**Database**” tab on the Search Settings dialog contains the following search parameters related to the database to be used for the Comet search:



- “**Proteome Database**” edit box corresponds to the “[database_name](#)” Comet search parameter.



- “**Target/Decoy/Decoy 1**” radio buttons correspond to the “[decoy_search](#)” parameter, and the “**Decoy Prefix**” edit box corresponding to the “[decoy_prefix](#)” parameter.

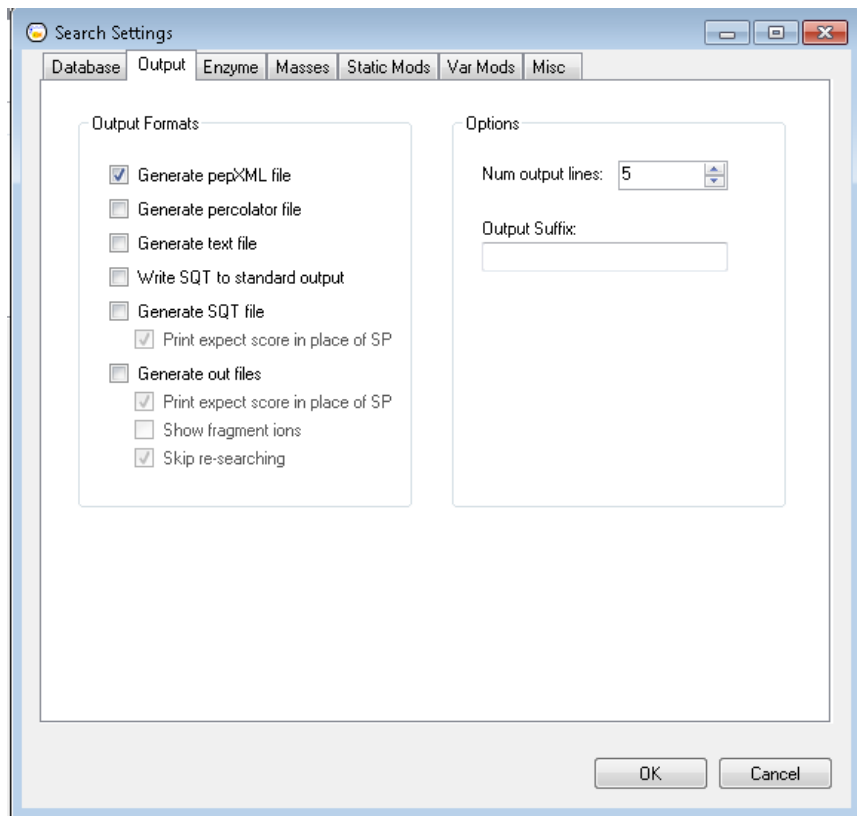


- “**Database Type**” drop-down corresponding to the “[nucleotide_reading_frame](#)” parameter.



Output Settings Tab

The “**Output**” tab on the Search Settings dialog contains the following search parameters related to the type of output generated by the Comet search:



- The following output format checkboxes correspond to the Comet search parameters indicated:
 - “Generate pepXML file” → [“output pepxmlfile”](#)
 - “Generate percolator file” → [“output percolatorfile”](#)
 - “Generate text file” → [“output txtfile”](#)
 - “Write SQT to standard output” → [“output sqtstream”](#)
 - “Generate SQT file” → [“output sqtfile”](#)
 - “Print expect score in place of SP” → [“print expect score”](#)
 - “Generate out files” → [“output outfiles”](#)
 - “Print expect score in place of SP” → [“print expect score”](#)
 - “Show fragment ions” → [“show fragment ions”](#)
 - “Skip researching” → [“skip researching”](#)
- The “Num of output lines” text box corresponds to the [“num output lines”](#) Comet search parameter.

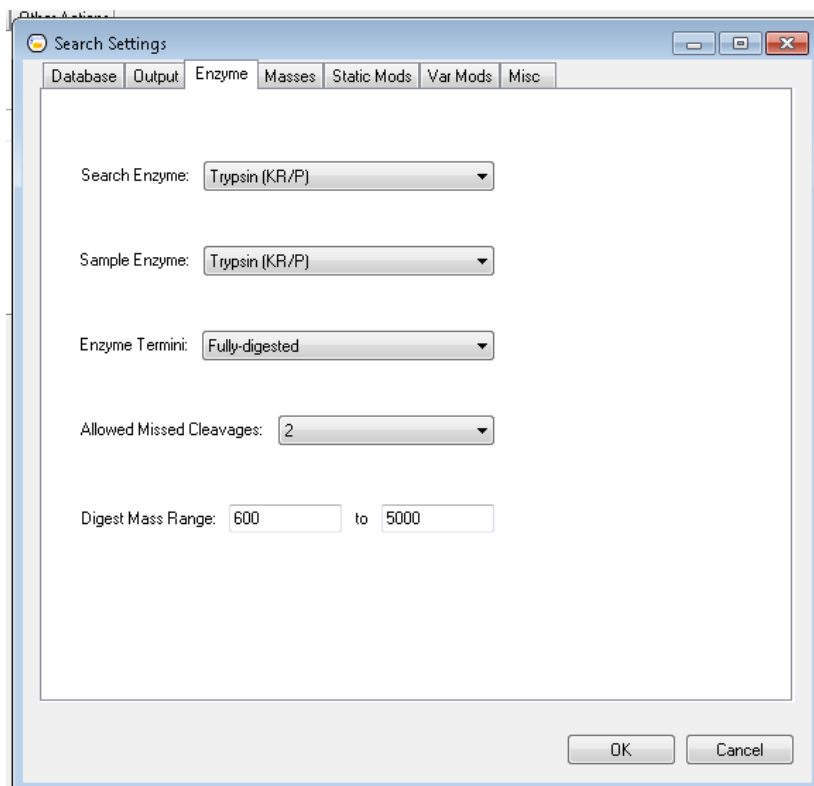
This is a close-up of the 'Options' section from the previous image, specifically the 'Num output lines' spinner box. It shows the number '5' in the text box with up and down arrow buttons on the right.

- The “**Output Suffix**” text box corresponds to the “[output suffix](#)” Comet search parameter.

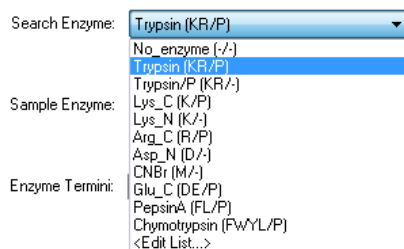
Output Suffix:

Enzyme Settings Tab

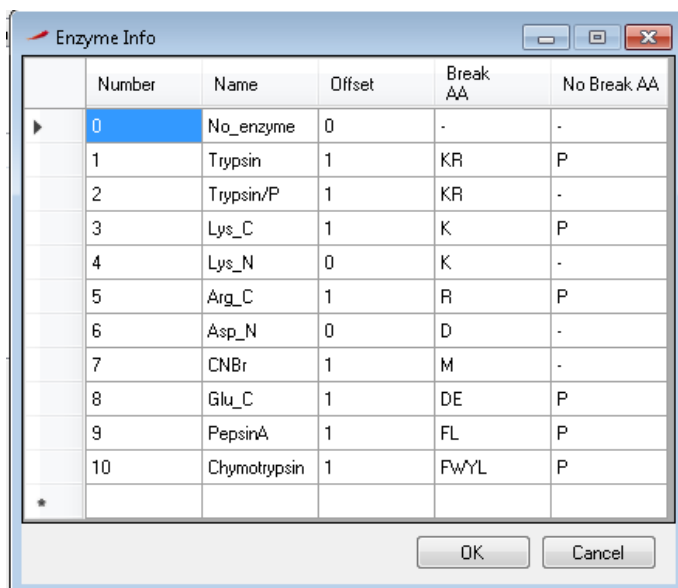
The “**Enzyme**” tab on the Search Settings dialog contains the following search parameters used in the Comet search:



- The “**Search Enzyme**” drop-down corresponds to the “[search enzyme number](#)” Comet search parameter:

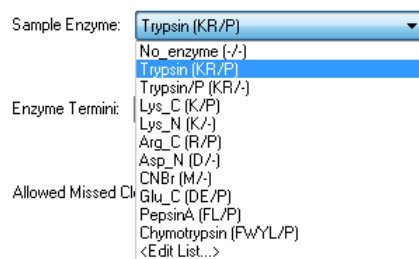


Clicking on the “<Edit List...>” item at the bottom of the drop-down list opens the following “**Enzyme Info**” dialog to allow users to edit the enzyme information listed in the drop down:



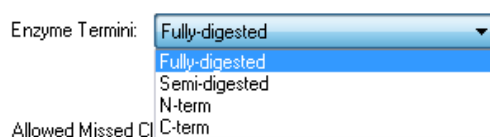
This dialog corresponds to the “[COMET_ENZYME_INFO]” list at the bottom of Comet “.params” files.

- The “Sample Enzyme” drop-down corresponds to the “[sample enzyme number](#)” Comet search parameter:



The “<Edit List...>” item opens up the same “Enzyme Info” dialog as above.

- The “Enzyme Termini” drop-down corresponds to the “[num enzyme termini](#)” Comet search parameter:



- The “Allowed Missed Cleavages” drop-down corresponds to the “[allowed missed cleavage](#)” Comet search parameter:

Allowed Missed Cleavages: 2

Digest Mass Range: 600

0
1
2
3
4
5
6
7
8
9
10

- The “**Digest Mass Range**” edit boxes correspond to the “[*digest mass range*](#)” Comet search parameter:

Digest Mass Range: 600 to 5000

Mass Settings Tab

The “**Masses**” tab on the Search Settings dialog contains precursor and fragment mass options used in the Comet search, such as mass units and tolerances:

Search Settings

Database
Output
Enzyme
Masses
Static Mods
Var Mods
Misc

Precursor

Mass Tol: ± 20

Mass Unit: ppm

Mass Type: mono

Isotope Error: C13 offsets

Tolerance Type: Apply to mass

Mass Offsets:

Fragment

Bin Size: 1.0005

Offset: 0.4

Mass Type: mono

Ions

☐ a

☐ x

☐ Flank

☒ b

☒ y

☒ Use NL

☐ c

☐ z

- The following “**Precursor**” mass options correspond to the Comet search parameters indicated:

Precursor

Mass Tol: Mass Unit:

Mass Type: Isotope Error:

Tolerance Type:

Mass Offsets:

- “Mass Tol” edit box → [“peptide mass tolerance”](#)
- “Mass Unit” drop-down → [“peptide mass units”](#)
- “Mass Type” drop-down → [“mass type parent”](#)
- “Isotope Error” drop-down → [“isotope error”](#)
- “Tolerance Type” drop-down → [“precursor tolerance type”](#)
- “Mass Offsets” edit box → [“mass offsets”](#)

- The following “**Fragment**” mass options correspond to the Comet search parameters indicated below:

Fragment

Bin Size: Offset:

Mass Type:

- “Offset” edit box → [“fragment bin offset”](#)
- “Mass Type” drop-down → [“mass type fragment”](#)
- “Bin Size” edit box → [“fragment bin tol”](#)

- The following “**Ions**” mass options correspond to the Comet search parameters indicated below:

Ions

☐ a ☐ x ☐ Flank

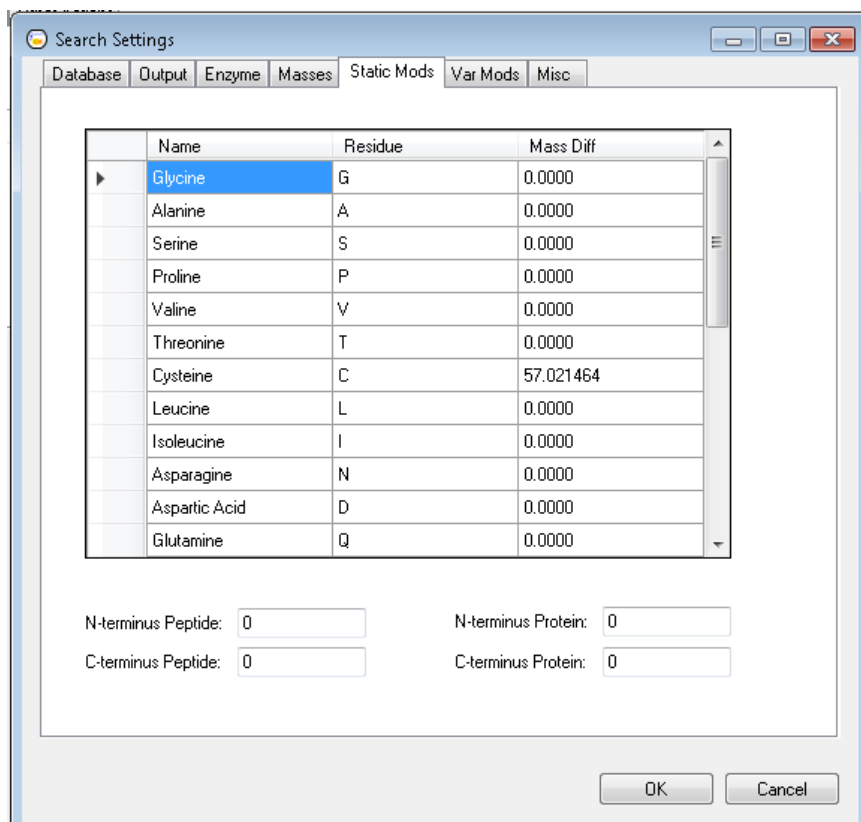
☒ b ☒ y ☒ Use NL

☐ c ☐ z

- “a” check box → [“use A ions”](#)
- “b” check box → [“use B ions”](#)
- “c” check box → [“use C ions”](#)
- “x” check box → [“use X ions”](#)
- “y” check box → [“use Y ions”](#)
- “z” check box → [“use Z ions”](#)
- “Use NL” check box → [“use NL ions”](#)

Static Mods Tab

The “**Static Mods**” tab on the Search Settings dialog contains static modification parameters used by the Comet search:



- The following table items correspond to the Comet search parameters indicated:

Name	Residue	Mass Diff
Glycine	G	0.0000
Alanine	A	0.0000
Serine	S	0.0000
Proline	P	0.0000
Valine	V	0.0000
Threonine	T	0.0000
Cysteine	C	57.021464
Leucine	L	0.0000
Isoleucine	I	0.0000
Asparagine	N	0.0000
Aspartic Acid	D	0.0000
Glutamine	Q	0.0000
Lysine	K	0.0000
Glutamic Acid	E	0.0000
Methionine	M	0.0000
Ornithine	O	0.0000
Histidine	H	0.0000
Phenylalanine	F	0.0000

- “Glycine” → “[add G glycine](#)”
- “Alanine” → “[add A alanine](#)”
- “Serine” → “[add S serine](#)”
- “Proline” → “[add P proline](#)”
- “Valine” → “[add V valine](#)”
- “Threonine” → “[add T threonine](#)”
- “Cysteine” → “[add C cysteine](#)”
- “Leucine” → “[add L leucine](#)”
- “Isoleucine” → “[add I isoleucine](#)”
- “Asparagine” → “[add N asparagine](#)”
- “Aspartic Acid” → “[add D aspartic acid](#)”
- “Glutamine” → “[add Q glutamine](#)”
- “Lysine” → “[add K lysine](#)”
- “Glutamic Acid” → “[add E glutamic acid](#)”
- “Methionine” → “[add M methionine](#)”
- “Ornithine” → “[add O ornithine](#)”
- “Histidine” → “[add H histidine](#)”
- “Phenylalanine” → “[add F phenylalanine](#)”

	Arginine	R	0.0000
	Tyrosine	Y	0.0000
	Tryptophan	W	0.0000
	User Amino Acid	B	0.0000
	User Amino Acid	J	0.0000
	User Amino Acid	U	0.0000
	User Amino Acid	X	0.0000
	User Amino Acid	Z	0.0000

- "Arginine" → ["add R arginine"](#)
- "Tyrosine" → ["add Y tyrosine"](#)
- "Tryptophan" → ["add W tryptophan"](#)
- "User Amino Acid (B)" → ["add B user amino acid"](#)
- "User Amino Acid (J)" → ["add J user amino acid"](#)
- "User Amino Acid (U)" → ["add U user amino acid"](#)
- "User Amino Acid (X)" → ["add X user amino acid"](#)
- "User Amino Acid (Z)" → ["add Z user amino acid"](#)

- The **"N-terminus Peptide"** text box corresponds to the ["add Nterm peptide"](#) parameter:

N-terminus Peptide:

- The **"C-terminus Peptide"** text box corresponds to the ["add Cterm peptide"](#) parameter:

C-terminus Peptide:

- The **"N-terminus Protein"** text box corresponds to the ["add Nterm protein"](#) parameter:

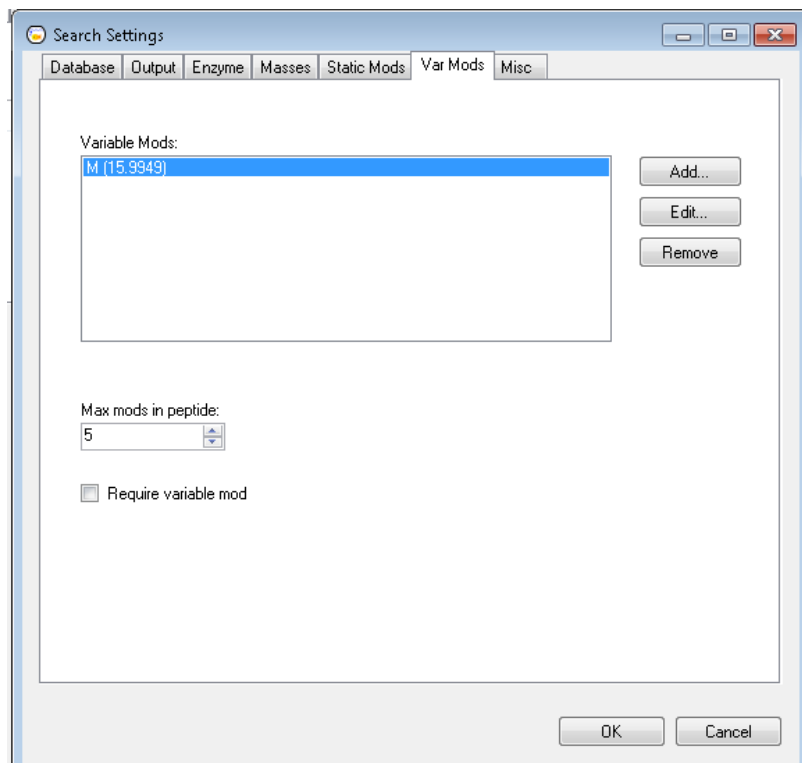
N-terminus Protein:

- The **"C-terminus Protein"** text box corresponds to the ["add Cterm protein"](#) parameter:

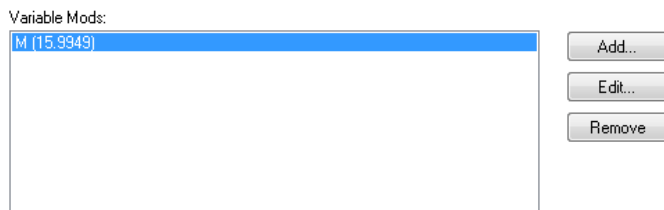
C-terminus Protein:

Var Mods Tab

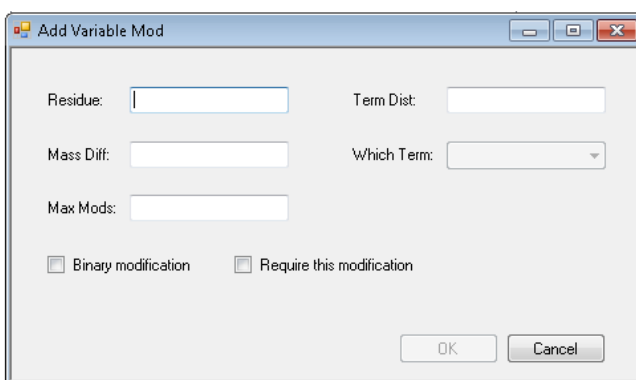
The **"Var Mods"** tab on the Search Settings dialog contains variable modification parameters used by the Comet search:



- The items in the “**Variable Mods**” list below correspond to the Comet variable mod parameters “[variable_mod0N](#)”, where N ranges from 0-9.



To add a variable modification, click on the “**Add...**” button on the right to open up the “**Add Variable Mod**” dialog below, and use this dialog to specify the various fields of the variable modification (these [variable mod fields](#) are described in more detail on the Comet website):



- The “**Residue**” text box corresponds to the second field on the variable mod parameter – the residue(s) that the modifications are possibly applied to.
- The “**Mass Diff**” text box corresponds to the first field on the variable mod parameter – specify the modification mass difference.
- The “**Max Mods**” text box corresponds to the fourth field on the variable mod parameter – specify the maximum number of modified residues possible in a peptide for this modification entry.
- The “**Binary modification**” check box corresponds to the third field on the variable mod parameter – specify whether the modification is a variable modification or a binary one.
- The “**Require this modification**” check box corresponds to the seventh field on the variable mod parameter – specify whether peptides must contain this modification.
- The “**Term Dist**” text box corresponds to the fifth field on the variable mod parameter – specify the distance the modification is applied to from the respective protein terminus.
- The “**Which Term**” drop-down corresponds to the sixth field on the variable mod parameter – specify which protein terminus the distance constraint is applied to.

To edit a variable mod, go back to the “**Variable Mods**” tab, select the variable mod item in the “**Variable Mods**” list and click on the “**Edit...**” button to open up the “**Edit Variable Mod**” dialog,

which is virtually identical to the “Add Variable Mod” dialog above, except with the fields populated to reflect the variable mod selected from the list.

To remove a variable mod from the “**Variable Mods**” list, just select the item and click on the “**Remove**” button.

- The “**Max Mods in Peptide**” text box corresponds to the “[max variable mods in peptide](#)” parameter:

Max mods in peptide:

- The “**Require variable mod**” check box corresponds to the “[require variable mod](#)” parameter:

☐ Require variable mod

Misc Tab

The “**Misc**” tab on the Search Settings dialog contains miscellaneous Comet search parameters:

The screenshot shows the "Search Settings" dialog box with the "Misc" tab selected. The dialog has several tabs: Database, Output, Enzyme, Masses, Static Mods, Var Mods, and Misc. The "Misc" tab contains two main sections: "mzXML" and "Spectral Processing".

mzXML Section:

- Scan Range: 0 to 0
- Precursor Charge: 0 to 0
- Override Charge: Keep known charges (dropdown)
- MS Level: 2 (dropdown)
- Activation Level: ALL (dropdown)

Spectral Processing Section:

- Min Peaks: 10
- Min Intensity: 0
- Precursor Removal Tol: ± 1.5
- Remove Precursor Peak: No (dropdown)
- Clear m/z Range: 0 to 0

Other Parameters:

- Spectrum Batch Size: 0
- Num Threads: 0 (dropdown)
- Num Results: 50
- Max Fragment Charge: 3 (dropdown)
- Max Precursor Charge: 6 (dropdown)
- ☐ Clip N-term methionine

At the bottom of the dialog are "OK" and "Cancel" buttons.

- The following “**mzXML**” fields correspond to the following Comet search parameters:

mzXML

Scan Range:
 to

Precursor Charge:
 to

Override Charge:

MS Level: Activation Level:

- “Scan Range” text boxes → [“scan_range”](#)
- “Precursor Charge” text boxes → [“precursor_charge”](#)
- “Override Charge” drop-down → [“override_charge”](#)
- “MS Level” drop-down → [“ms_level”](#)
- “Activation Level” text boxes → [“activation_method”](#)

- The following “**Spectral Processing**” fields correspond to the following Comet search parameters:

Spectral Processing

Min Peaks: Min Intensity:

Precursor Removal Tol: ±

Remove Precursor Peak:

Clear m/z Range:
 to

- “Min Peaks” text box → [“minimum_peaks”](#)
- “Min Intensity” text box → [“minimum_intensity”](#)
- “Precursor Removal Tol” text box → [“remove_precursor_tolerance”](#)
- “Remove Precursor Peak” drop-down → [“remove_precursor_peak”](#)
- “Clear m/z Range” text boxes → [“clear_mz_range”](#)

- The rest of the miscellaneous parameters correspond to the following Comet search parameters:

Spectrum Batch Size: Max Fragment Charge:

Num Threads: Num Results: Max Precursor Charge:

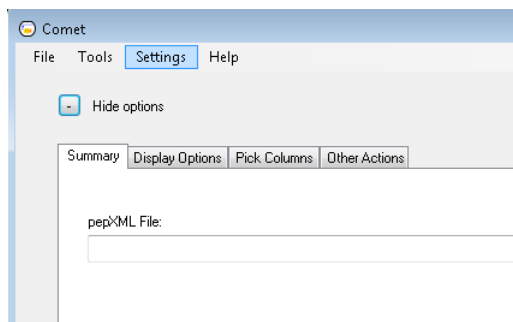
☐ Clip N-term methionine

- The “**Spectrum Batch Size**” text box corresponds to the [“spectrum_batch_size”](#) parameter.
- The “**Num Threads**” drop-down corresponds to the [“num_threads”](#) parameter.
- The “**Num Results**” text box corresponds to the [“num_results”](#) parameter.
- The “**Max Fragment Charge**” drop-down corresponds to the [“max_fragment_charge”](#) parameter.
- The “**Max Precursor Charge**” drop-down corresponds to the [“max_precursor_charge”](#) parameter.
- The “**Clip N-term methionine**” checkbox corresponds to the [“clip_nterm_methionine”](#) parameter.

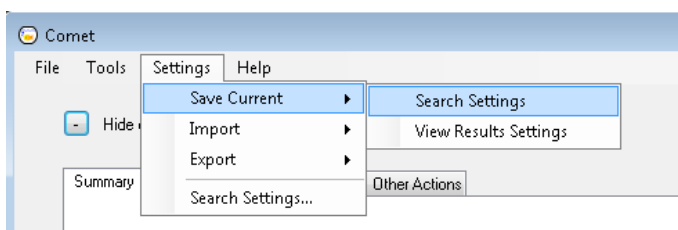
Save Search Settings

To save any changes made to the search settings:

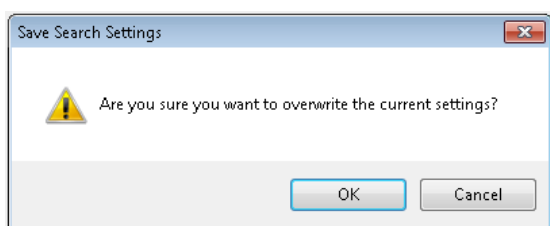
1. Click on the **“Settings”** menu:



2. Choose the **“Save Current... → Search Settings”** menu item:

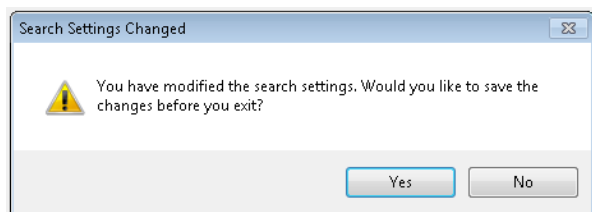


3. Click on the **“OK”** button on the confirmation dialog that pops up:



Now, if the CometUI application is rebooted, the changes made to the search settings will be preserved.

Alternatively, if changes were made to the search settings, and the user tries to close the CometUI application without saving these changes, the following dialog will appear giving the user a chance to save the changes by clicking on the **“Yes”** button.



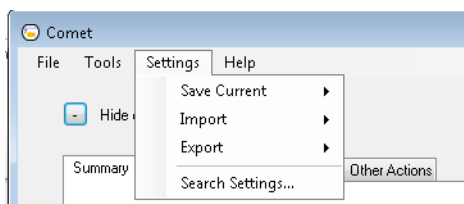
Import/Export Search Settings

The CometUI application allows users to import Comet search settings from a “.params” Comet parameter file, as well as export the settings in the UI to a “.params” file.

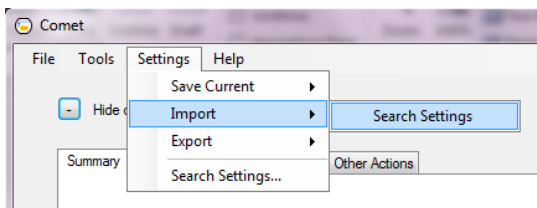
Import Search Settings

To import the search settings:

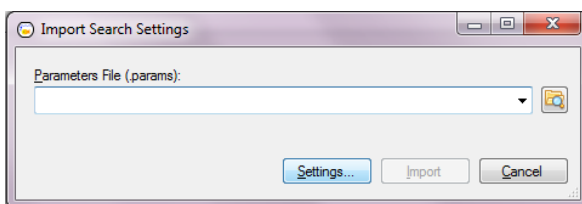
1. Click on the **“Settings”** menu:



2. Choose the **“Import → Search Settings”** menu item:

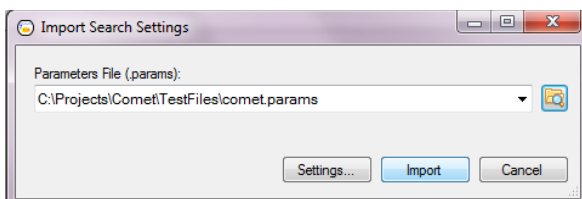


3. The following **“Import Search Settings”** dialog should open up:



Note: The **“Settings...”** button can be used to view the current settings in CometUI.

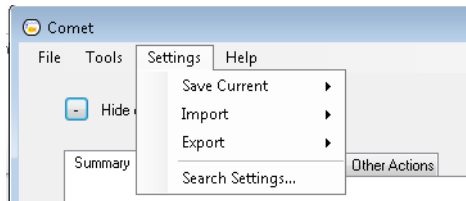
4. Use the folder browse button on this dialog to browse to the **“.params”** file to be imported, and click on the **“Import”** button:



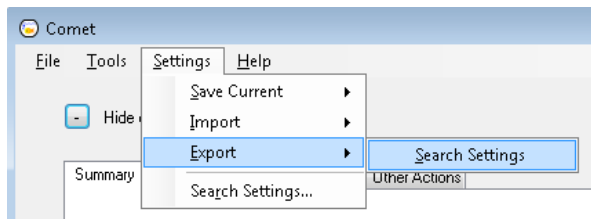
Export Search Settings

To export the search settings:

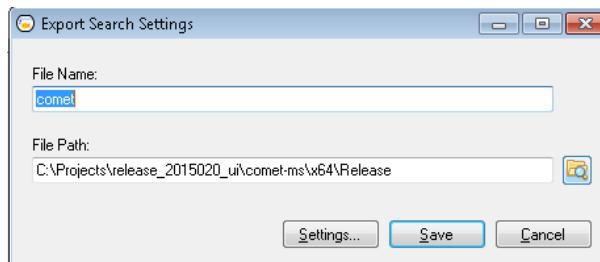
1. Click on the **“Settings”** menu:



2. Choose the **“Export → Search Settings”** menu item:

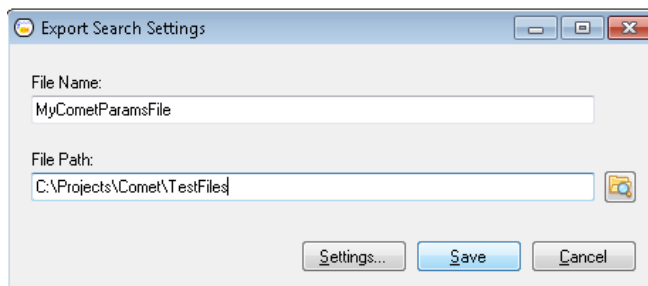


3. The following **“Export Search Settings”** dialog should open up:



Note: The **“Settings...”** button can be used to view/edit the current settings.

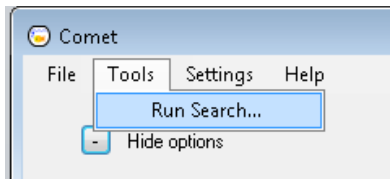
4. Choose a **“File Name”** (default is “comet”), a **“File Path”** (default is the current directory the CometUI.exe is running in) and click on the **“Save”** button, and the exported “.params” file with the specified name will get saved in specified location:



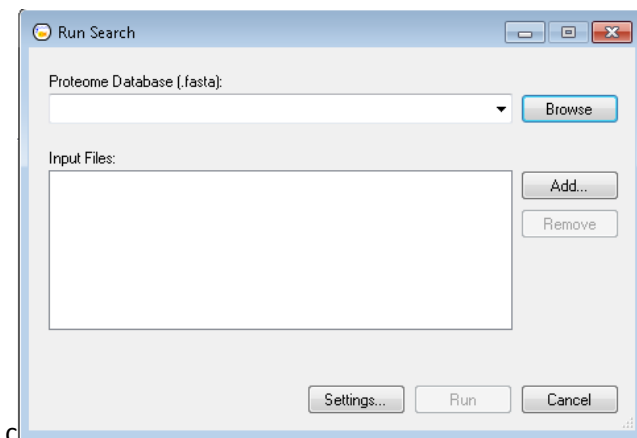
Run Search

CometUI provides the user with a graphical user interface to run the Comet search engine. To run a search:

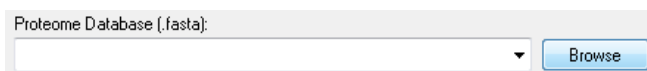
1. Click on the “Tools” menu and select the “Run Search...” menu item:



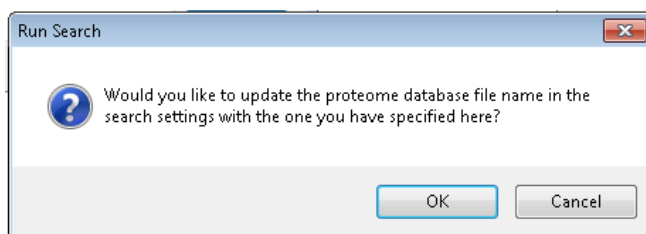
2. This will bring up the following window:



3. Specify a “**Proteome Database (.fasta)**” file using the “**Browse**” button:



If the file specified is different than the one in the search settings, the following message box will pop up:



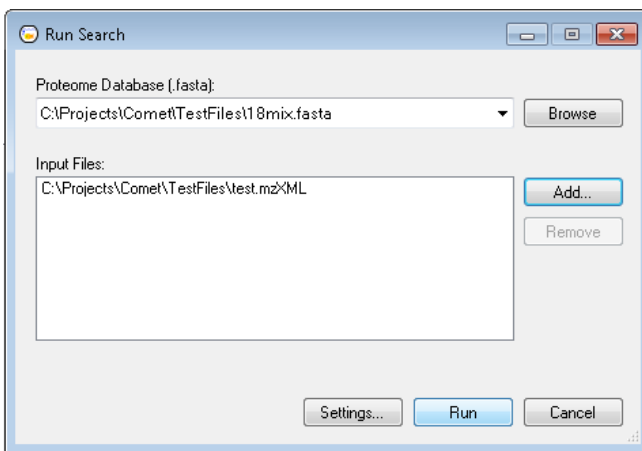
Click “**OK**” to update the proteome database file name in the search settings to this file, or “**Cancel**” to leave the search settings unchanged.

- Next, click on the **“Add...”** button next to the **“Input Files”** list box to specify an input file (or multiple input files):

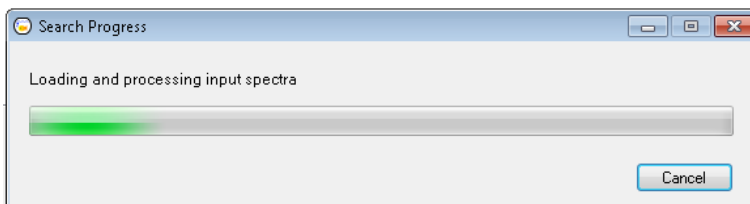


Formats currently supported are: “.mgf”, “.mzxml”, “.mzml”, “.ms2”, “.cms2” and “.raw”.

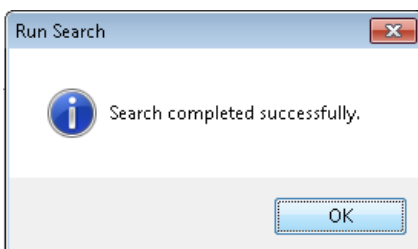
- Once at least one input file has been added, the **“Run”** button will become active:



- Clicking the **“Run”** button will launch the search, and a **“Search Progress”** dialog should appear:



- If the search completes successfully, the notification below should appear, and clicking **“OK”** on it should bring up the results automatically in the results viewer, which will be discussed next. (Note that if multiple input files were specified, only the results of the **FIRST** file in the list will be displayed in the results viewer.)



8. The results in the results viewer may look something like the following:

Comet

File Tools Settings Help

☐ Hide options

Summary Display Options Pick Columns Other Actions

pepXML File:
C:\Projects\Comet\TestFiles\test.pep.xml

Trypsin digest, Comet search engine, quantitation: [none]

Displaying 1996 of 1996 total spectra.

Update

SPECTRUM	SS...	EXPECT	IONS	PEPTIDE	PROTEIN	CALC_MASS
test.00005.00005.2	5	999	2/20	R.TQINKVRFDK.L	P01012DVAL_CHICK	1346.767034
test.00006.00006.2	6	17.3	4/24	K.VLGNPSNEEMNAK.K	P02602MLE1_RABIT	1401.655829
test.00272.00272.3	272	223	5/132	R.C160.03PETLFPSPFSGMESAGIHETTYNSIMKCT160.03DIDIR.K	P62739ACTA_BOVIN	3959.820218
test.00323.00323.2	323	287	4/28	R.WLPAM147.04SERVTRM147.04VQR.D	P00722B GAL_ECOLI	1890.955627
test.00331.00331.2	331	999	2/36	K.AVGKVIPELNGKLTGMAFR.V	P46406G3P_RABIT	2000.124102
test.00376.00376.2	376	999	0/40	R.FNDDFSRAVLEAEVQM147.04C160.03GELR.D	P00722B GAL_ECOLI	2501.131494
test.00410.00410.3	410	668	2/104	R.HMNGYGSHTKLVNANGEAVYC160.03KFHYK.T	P00432CATA_BOVIN	3171.480729
test.00520.00520.2	520	83.3	3/30	-M147.04QKLVSVQNYAWGSK.T	P00946MANA_ECOLI	1881.940703
test.00550.00550.3	550	999	4/108	R.IGLNC160.03QAQVAERVNWLGLGPQENYFDR.L	P00722B GAL_ECOLI	3209.604016
test.00619.00619.2	619	999	2/46	K.MIKLITAIGDVNHDPPVGDRLR.V	P00489PYGM_RABIT	2643.489427
test.00629.00629.2	629	871	1/20	K.RLC160.03ENIAGHLK.D	P00432CATA_BOVIN	1309.692489
test.00652.00652.3	652	605	4/104	R.VTEQESKPVQM147.04M147.04YQIGLFRVASMASEK.M	P01012DVAL_CHICK	3118.513699
test.00658.00658.3	658	999	6/80	K.WGDAGAEYVVESTGVFTTMEK.A	P46406G3P_RABIT	2276.030715
test.00870.00870.3	870	999	4/100	K.HSTVFDNLPNPDPRKNYELLCT160.036DNTR.K	Q29443TRFE_BOVIN	3103.441761
test.00985.00985.3	985	442	6/80	R.YYGYTGAFRC160.03LVEKGDVAFVK.D	Q29443TRFE_BOVIN	2442.204203
test.00987.00987.3	987	999	0/92	R.ESKPPDSSKDEC160.03M147.04VKWC160.03AIGHQER.T	Q29443TRFE_BOVIN	2889.284383
test.01046.01046.3	1046	286	4/92	K.TYDSYLGDDYVRAMTNLRQC160.03STSK.L	Q29443TRFE_BOVIN	2843.285443
test.01114.01114.2	1114	434	3/32	K.C160.03ACT160.03SNHEPYFGYSGAFK.C	Q29443TRFE_BOVIN	1993.808718
test.01204.01204.3	1204	999	1/104	-MTM147.04ITDGLAVLQRRDWENPGVTQLNR.L	P00722B GAL_ECOLI	3158.596473
test.01345.01345.2	1345	240	1/42	K.IVNANGFAYYC160.03KFHYKTDGRIK.N	P00432CATA_BOVIN	2554.263844