



Comet UI

User Guide

Comet UI Version 1.0.0.0

Comet Search Engine Version 2015.02 rev. 0

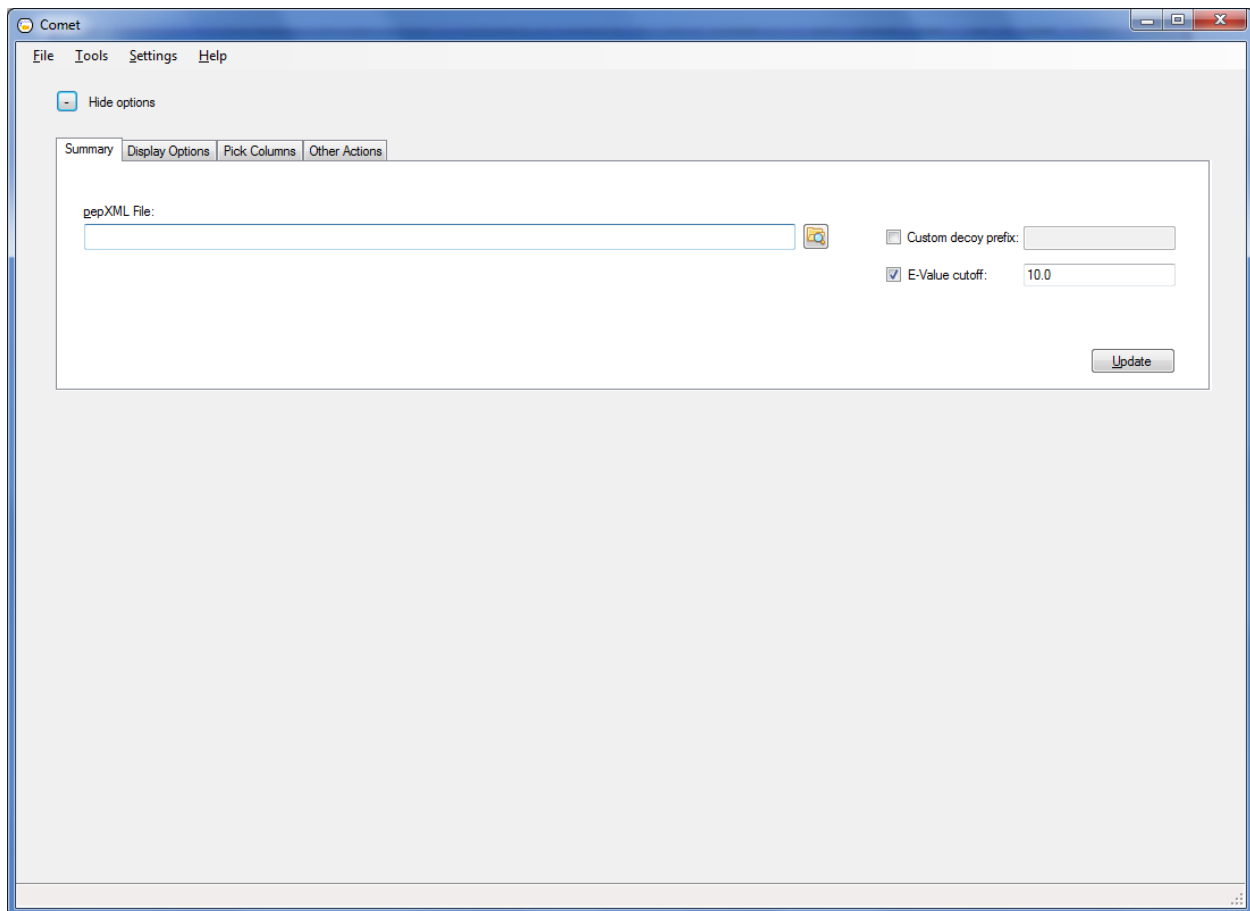
Contents

Introduction	3
View and Edit Search Settings.....	4
Database Search Settings Tab	5
Output Settings Tab	6
Enzyme Settings Tab	7
Mass Settings Tab	9
Static Mods Tab.....	11
Var Mods Tab	12
Misc Tab	14
Save Search Settings	16
Import/Export Search Settings.....	17
Import Search Settings.....	17
Export Search Settings	18
Run Search	19
View Results.....	22

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:



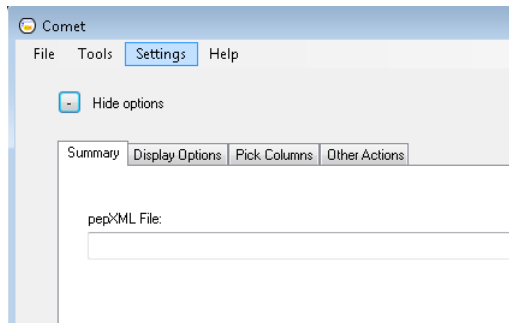
This document will describe how to navigate this window to perform the following tasks:

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

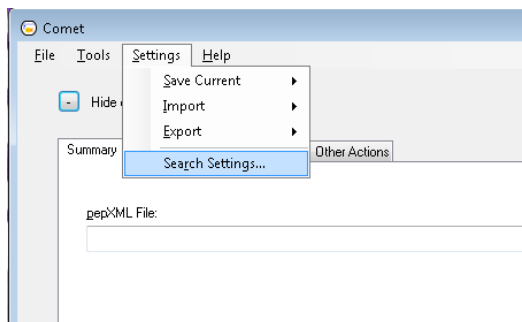
View and Edit Search Settings

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:

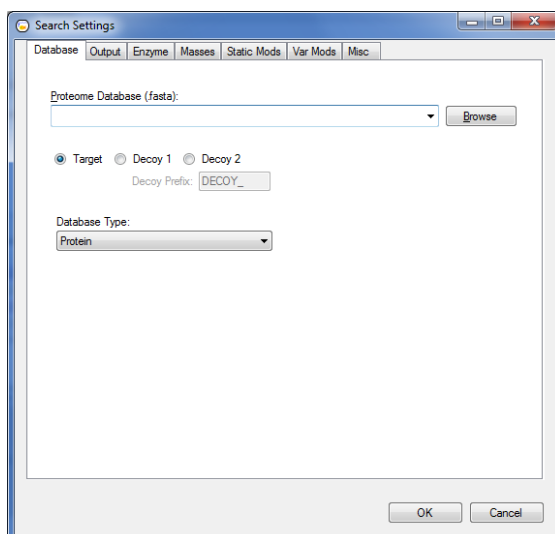
1. Click on the “**Settings**” menu:



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

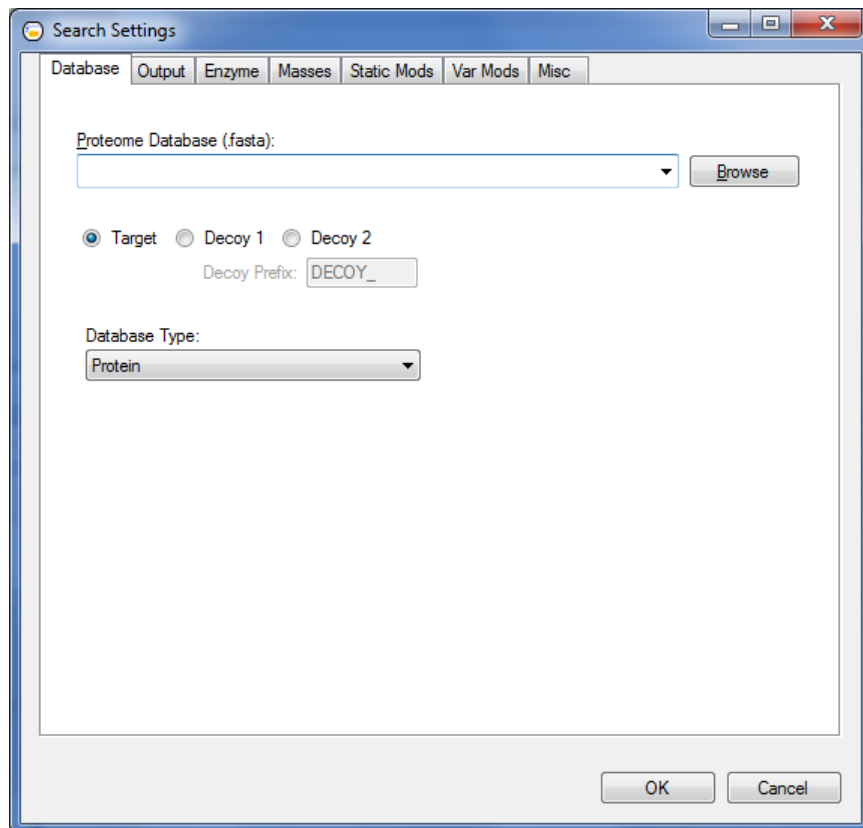


3. The following dialog should open up:



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:



The screenshot shows the 'Search Settings' dialog box with the 'Database' tab selected. The dialog has a title bar with standard window controls. Below the title bar are tabs for 'Database', 'Output', 'Enzyme', 'Masses', 'Static Mods', 'Var Mods', and 'Misc'. The 'Database' tab contains the following controls: a 'Proteome Database (fasta):' label above a text box with a dropdown arrow and a 'Browse' button; three radio buttons labeled 'Target', 'Decoy 1', and 'Decoy 2', with 'Target' selected; a 'Decoy Prefix:' label above a text box containing 'DECOY_'; a 'Database Type:' label above a dropdown menu showing 'Protein'; and 'OK' and 'Cancel' buttons at the bottom right.

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



This detail shows the 'Proteome Database (fasta):' label, a text box with a dropdown arrow, and a 'Browse' button.

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



This detail shows the three radio buttons labeled 'Target', 'Decoy 1', and 'Decoy 2', with 'Target' selected. Below them is the 'Decoy Prefix:' label and a text box containing 'DECOY_'.

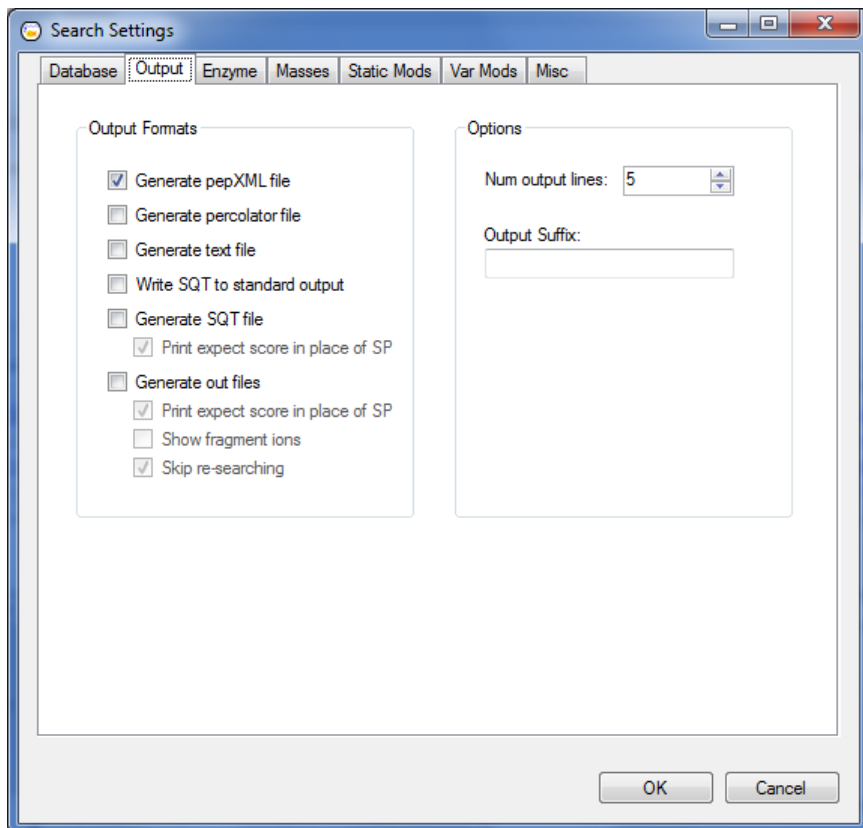
- “**Database Type**” drop-down corresponding to the “[nucleotide_reading_frame](#)” parameter.



This detail shows the 'Database Type:' label and a dropdown menu showing 'Protein'.

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 re-searching” → “[skip researching](#)”
- The “Num of output lines” text box corresponds to the “[num output lines](#)” Comet search parameter.

Options

Num output lines:

- 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:

Search Settings

Database Output **Enzyme** Masses Static Mods Var Mods Misc

Search Enzyme: Trypsin (KR/P)

Sample Enzyme: Trypsin (KR/P)

Enzyme Termini: Fully-digested

Allowed Missed Cleavages: 2

Digest Mass Range: 600 to 5000

OK Cancel

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

Search Enzyme: **Trypsin (KR/P)**

Sample Enzyme:

Enzyme Termini:

<Edit List...>

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:

Enzyme Info

	Number	Name	Offset	Break AA	No Break AA
▶	0	No_enzyme	0	-	-
	1	Trypsin	1	KR	P
	2	Trypsin/P	1	KR	-
	3	Lys_C	1	K	P
	4	Lys_N	0	K	-
	5	Arg_C	1	R	P
	6	Asp_N	0	D	-
	7	CNBr	1	M	-
	8	Glu_C	1	DE	P
	9	PepsinA	1	FL	P
	10	Chymotrypsin	1	FWYL	P
*					

OK Cancel

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:

Sample Enzyme: **Trypsin (KR/P)**

Enzyme Termini:

Allowed Missed Cl:

<Edit List...>

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:

Enzyme Termini: **Fully-digested**

Allowed Missed Cleavages: **Fully-digested**

Allowed Missed Cleavages: **Semi-digested**

Allowed Missed Cleavages: **N-term**

Allowed Missed Cleavages: **C-term**

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

Allowed Missed Cleavages: **2**

Digest Mass Range: **600**

Digest Mass Range: **3**

Digest Mass Range: **4**

Digest Mass Range: **5**

Digest Mass Range: **6**

Digest Mass Range: **7**

Digest Mass Range: **8**

Digest Mass Range: **9**

Digest Mass Range: **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

OK Cancel

- 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

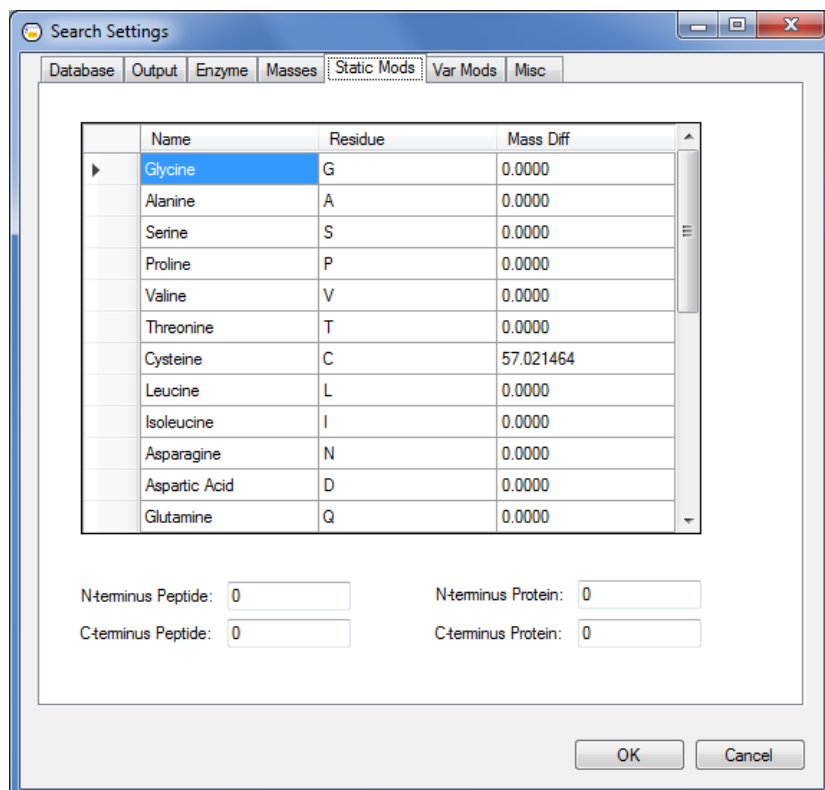
☒ b ☒ y ☒ Use NL

☐ 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:

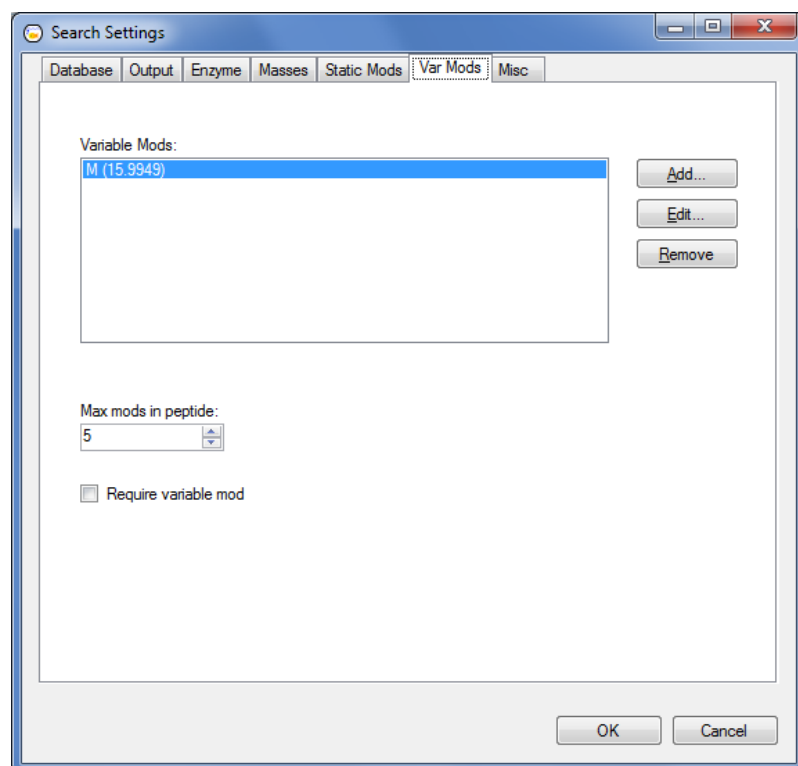
N-terminus Protein:

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

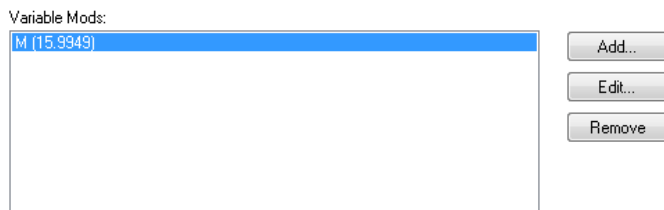
C-terminus Protein:

Var Mods Tab

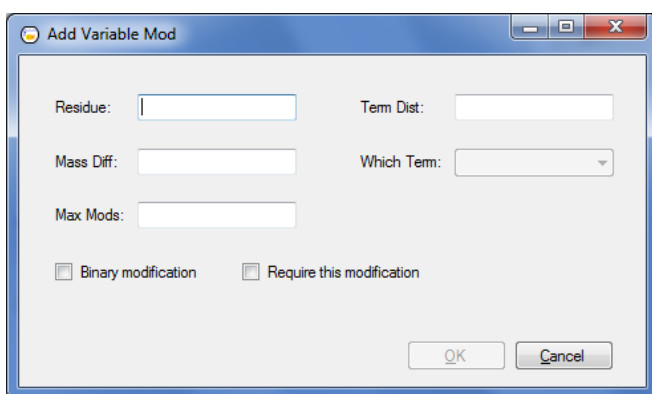
The **"Var Mods"** tab on the Search Settings dialog contains variable modification parameters used by the Comet search:



- 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

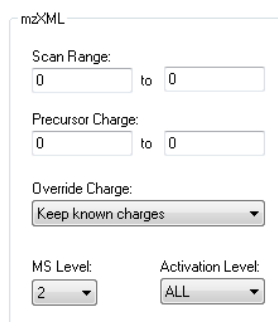
Misc Tab

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 is divided into two main sections: 'mzXML' and 'Spectral Processing'. The 'mzXML' section includes fields for 'Scan Range' (0 to 0), 'Precursor Charge' (0 to 0), 'Override Charge' (Keep known charges), 'MS Level' (2), and 'Activation Level' (ALL). The 'Spectral Processing' section includes fields for 'Min Peaks' (10), 'Min Intensity' (0), 'Precursor Removal Tol' (± 1.5), 'Remove Precursor Peak' (No), and 'Clear m/z Range' (0 to 0). At the bottom, there are fields for 'Spectrum Batch Size' (0), 'Num Threads' (0), 'Num Results' (50), 'Max Fragment Charge' (3), 'Max Precursor Charge' (6), and a checkbox for 'Clip N-term methionine'. The 'OK' and 'Cancel' buttons are at the bottom right.

Section	Parameter	Value
mzXML	Scan Range	0 to 0
	Precursor Charge	0 to 0
	Override Charge	Keep known charges
	MS Level	2
	Activation Level	ALL
Spectral Processing	Min Peaks	10
	Min Intensity	0
	Precursor Removal Tol	± 1.5
	Remove Precursor Peak	No
	Clear m/z Range	0 to 0
Bottom Section	Spectrum Batch Size	0
	Num Threads	0
	Num Results	50
	Max Fragment Charge	3
	Max Precursor Charge	6
Clip N-term methionine		<input type="checkbox"/>

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



mzXML

Scan Range: 0 to 0

Precursor Charge: 0 to 0

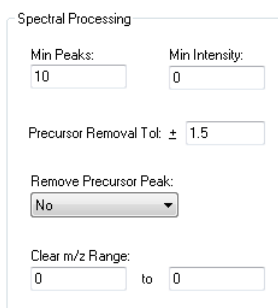
Override Charge: Keep known charges

MS Level: 2

Activation Level: ALL

- “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: 10

Min Intensity: 0

Precursor Removal Tol: ± 1.5

Remove Precursor Peak: No

Clear m/z Range: 0 to 0

- “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: 0

Num Threads: 0

Num Results: 50

Max Fragment Charge: 3

Max Precursor Charge: 6

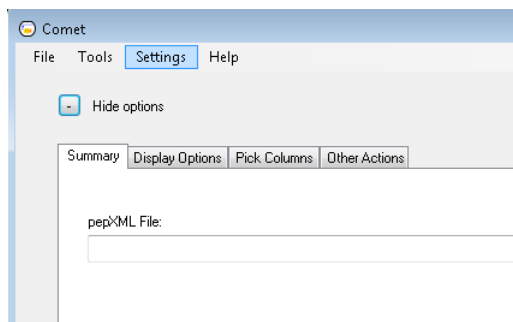
☐ Clip N-term methionine

- 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.

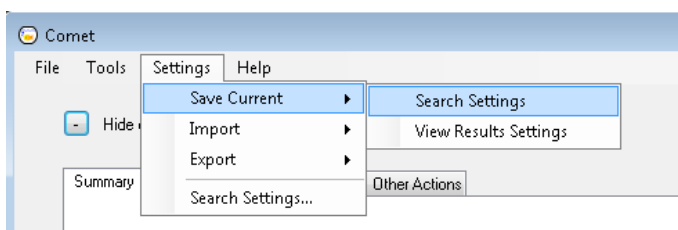
Save Search Settings

To save any changes made to the search settings:

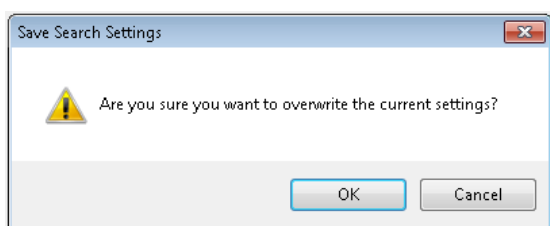
1. Click on the **“Settings”** menu:



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

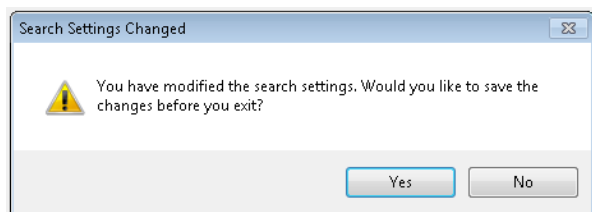


3. Click on the **“OK”** button on the confirmation dialog that pops up:



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.



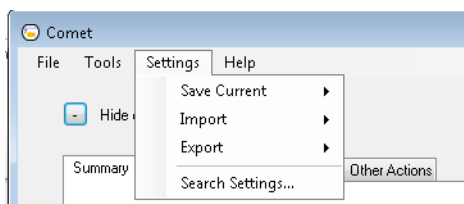
Import/Export Search Settings

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.

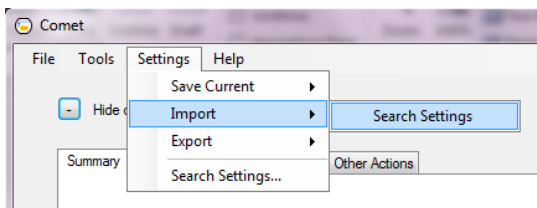
Import Search Settings

To import the search settings:

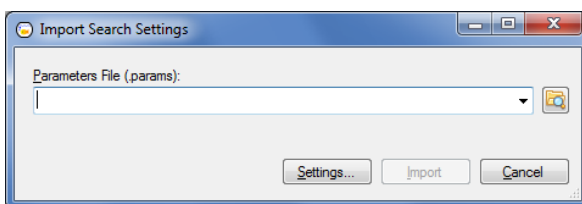
1. Click on the **“Settings”** menu:



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

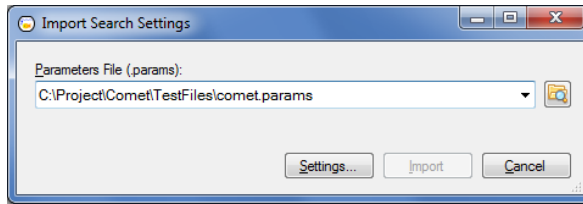


3. The following **“Import Search Settings”** dialog should open up:



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

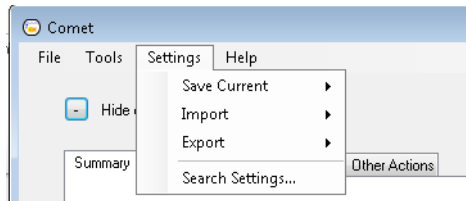
4. Use the folder browse button on this dialog to browse to the **“.params”** file to be imported, and click on the **“Import”** button:



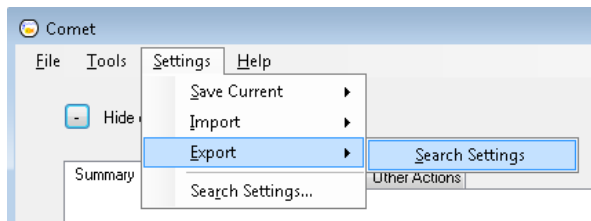
Export Search Settings

To export the search settings:

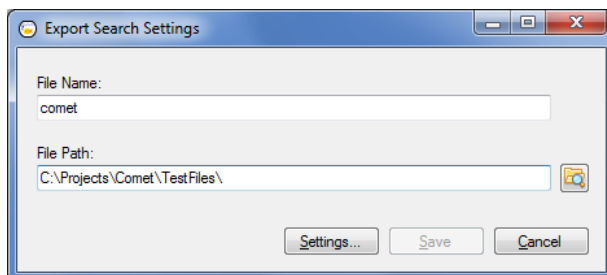
1. Click on the **“Settings”** menu:



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

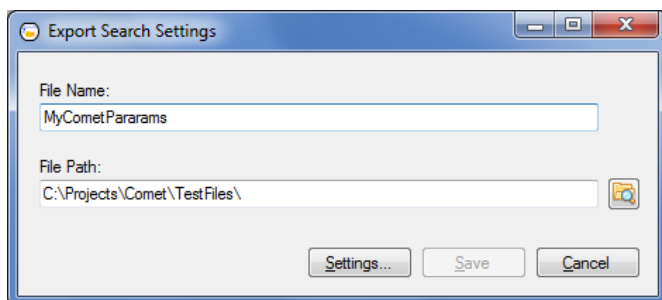


3. The following **“Export Search Settings”** dialog should open up:



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

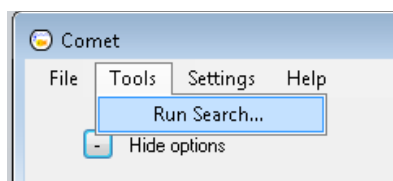
4. Choose a **“File Name”** (default is “comet”), a **“File Path”** (default is the current directory the CometUI.exe is running in) and click on the **“Save”** button, and the exported “.params” file with the specified name will get saved in specified location:



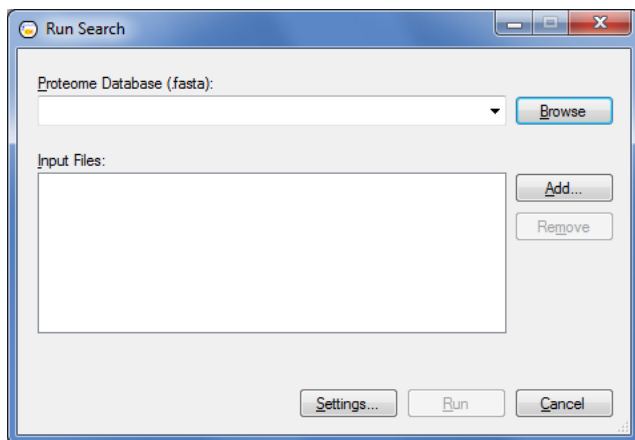
Run Search

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

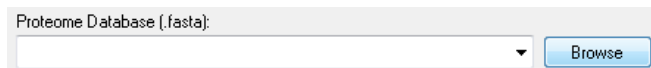
1. Click on the “Tools” menu and select the “Run Search...” menu item:



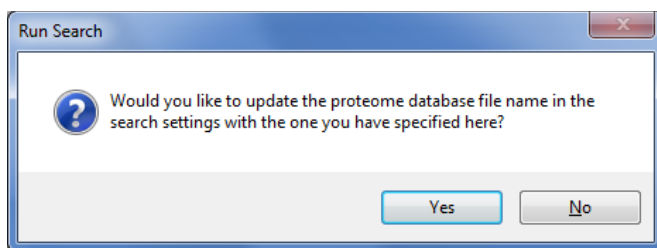
2. This will bring up the following window:



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:



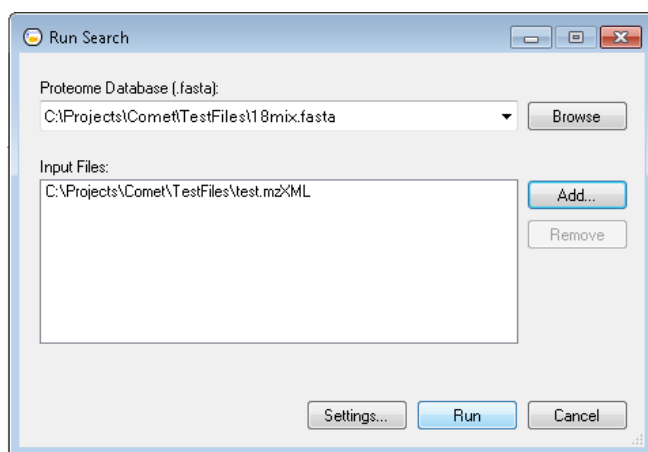
Click **"OK"** to update the proteome database file name in the search settings to this file, or **"Cancel"** to leave the search settings unchanged.

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

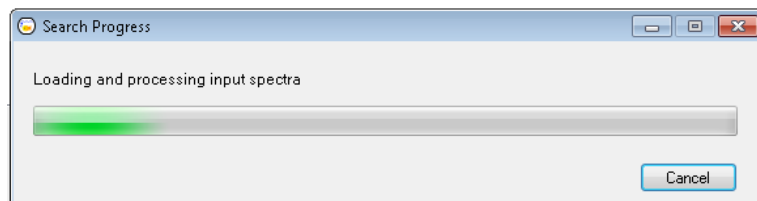


Formats currently supported are: ".mgf", ".mzxml", ".mzml", ".ms2", ".cms2" and ".raw".

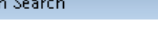
5. Once at least one input file has been added, the **"Run"** button will become active:



6. Clicking the **"Run"** button will launch the search, and a **"Search Progress"** dialog should appear:



7. 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.



File

Tools

Settings

Help

Hide options

Summary

Display Options

Pick Columns

Other Actions

gpxXML File:

C:\Users\engi\Desktop\search20150602_UC_pool_DDA_02.pep.xml

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

Displaying 82395 of 82395 total spectra.

☐ Custom decay prefix:

☐ E/Value cutoff: 10.0

Update

SPECTRUM	SCAN	EXPECT	IONS	PEPTIDE	PROTEIN	CALC_MASS
20150602_UC_poo1_DDA_02.11617.11617.3	11617	2.68E-14	43/156	R.GCSCGSHGCGSGFGSGCGSYGGEEASGCGGYYGCGSK.S	tr K17E003 K17E003_HUMAN	3222.274297
20150602_UC_poo1_DDA_02.34430.34430.3	34430	1.04E-13	35/112	K.VADALTNNAVHVDMM147.04PNALSLDLHAHK.L	tr G3V1N2 G3V1N2_HUMAN	3011.447069
20150602_UC_poo1_DDA_02.43967.43967.7	43967	4.45E-13	39/120	K.QQVETQAQAEVSAAGAAQVVDQATEQSK.A	sp Q15847 ADIRF_HUMAN	3040.46975
20150602_UC_poo1_DDA_02.18121.18121.3	18121	6.45E-13	43/96	R.LHVLHLYTPQGETINCD160.03EQCL60.03VC160.03NACR.W	sp Q02817 MUC2_HUMAN	2928.270145
20150602_UC_poo1_DDA_02.33712.33712.2	33712	1.53E-12	38/84	R.LVRPEVDVMC160.03TAFHNDTEFLK.K	tr A0A087WMT3 A0A08..._HUMAN	2649.256709
20150602_UC_poo1_DDA_02.18300.18300.3	18300	1.93E-12	37/96	R.LHGLHLYTPQGETINCD160.03EQCL60.03VC160.03NACR.W	sp Q02817 MUC2_HUMAN	2928.270145
20150602_UC_poo1_DDA_02.33898.33898.8	33898	2.26E-12	37/84	R.LVRPEVDVMC160.03TAFHNDTEFLK.K	tr A0A087WMT3 A0A08..._HUMAN	2649.256709
20150602_UC_poo1_DDA_02.43966.43966.2	43966	2.63E-12	34/42	R.KPLVITAEVDGDEALSTLVNLR.L	sp P10809 CHMO_HUMAN	2364.326427
20150602_UC_poo1_DDA_02.16726.16726.2	16726	2.67E-12	29/52	K.ASASGCGAGVQPTTSGSSGASSVTVTR.S	sp P02541 LMBL_HUMAN	2364.15171
20150602_UC_poo1_DDA_02.53036.53036.2	53036	3.24E-12	34/44	K.HLVMLGIVPAWVAHDAEALGK.K	tr E8P186 EP8P186_HUMAN	2351.230752
20150602_UC_poo1_DDA_02.40081.40081.3	40081	3.72E-12	43/132	R.MCYAEAPDAVTHGAAPAVPVEELQDK.KPCGR.L	tr F55806 F55806_HUMAN	3503.787125
20150602_UC_poo1_DDA_02.42763.42763.3	42763	5.04E-12	40/116	K.TTTPTEEEEEEAAAGVVEELPHQQTGR.A	sp P20700 LMBL_HUMAN	3410.563769
20150602_UC_poo1_DDA_02.25734.25734.3	25734	6.34E-12	32/112	R.QSGQTDPLQKELQSGVDAANSAAQYQR.R	sp P46940 TQCA1_HUMAN	3146.486462
20150602_UC_poo1_DDA_02.43191.43191.3	43191	6.91E-12	41/116	K.TTTPTEEEEEEAAAGVVEELPHQQTGR.A	sp P20700 LMBL_HUMAN	3410.563769
20150602_UC_poo1_DDA_02.10197.10197.2	10197	8.53E-12	26/60	R.GGGGCGGCGSGSYSGCGGSGGGGGGGR.G	sp P04264 K1_HUMAN	2382.944571
20150602_UC_poo1_DDA_02.43754.43754.4	43754	9.69E-12	32/112	R.DVNVINLHATAGTVAAGVSGGSENVK.R	sp P51930 QCR1_HUMAN	3129.551983
20150602_UC_poo1_DDA_02.38185.38185.3	38185	1.03E-11	48/116	K.KVADALTNNAVHVDMPNALSLDLHAHK.L	tr G3V1N2 G3V1N2_HUMAN	3123.577312
20150602_UC_poo1_DDA_02.10621.10621.2	10621	1.22E-11	26/40	R.NPSSASGSSGSSGSGPGSTQNR.N	sp P02671 FIBA_HUMAN	1962.841609
20150602_UC_poo1_DDA_02.17399.17399.2	17399	1.39E-11	27/48	R.NMGCPYGGYGGGSGGSGGGGCGYR.S	sp P22626 ROZD_HUMAN	2188.898078
20150602_UC_poo1_DDA_02.38138.38138.3	38138	1.63E-11	40/92	K.HISQTSIVAEADDESLHLLGVCK.K	sp P49773 HINTL1_HUMAN	2605.305768
20150602_UC_poo1_DDA_02.30699.30699.3	30699	1.69E-11	42/24	K.AHNPASGASTCE160.03VTPHDAQYVETPFYFK.G	tr E7E095 E7E095_HUMAN	3518.557244
20150602_UC_poo1_DDA_02.29772.29772.3	29772	1.79E-11	39/116	R.LSLEADSHM160.03LEGAPVVDQATEQSK.160.03CCL60.03PDHFLDEK.G	sp Q02817 MUC2_HUMAN	3449.396393
20150602_UC_poo1_DDA_02.35365.35365.2	35365	2.51E-11	29/30	K.HQAAVEELTQLEQFK.R	tr B1P543 B1P543_HUMAN	1809.937407
20150602_UC_poo1_DDA_02.51145.51145.3	51145	2.61E-11	38/124	K.VLDINDEINPVFTQGVGVSEELSAHTLVK.I	sp P02541 LMBL_HUMAN	3515.749402
20150602_UC_poo1_DDA_02.11828.11828.3	11828	2.76E-11	48/152	R.GCSCGSHGCGSGGSGCGGGGSGGSGGSGGYR.G	sp P04264 K1_HUMAN	3311.300846
20150602_UC_poo1_DDA_02.18035.18035.3	18035	2.94E-11	36/96	R.LHGLHLYTPQGETINCD160.03EQCL60.03VC160.03NACR.W	sp Q02817 MUC2_HUMAN	2928.270145
20150602_UC_poo1_DDA_02.30243.30243.3	30243	3.09E-11	39/124	K.ASAGHVSIAQDAGADGWDTDPDYNVSEK.E	sp Q14247 Q14247_HUMAN	3331.438903
20150602_UC_poo1_DDA_0						

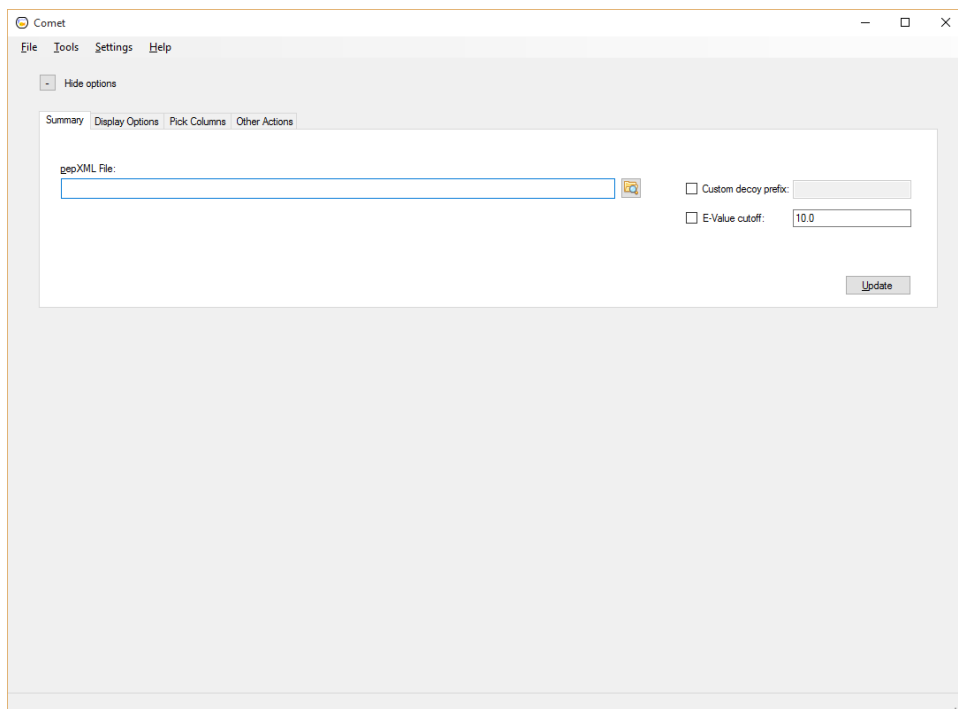
View Results

CometUI allows users to visualize Comet search results. Currently, only Comet searches generating a “*pep.xml*” file can be viewed in the results viewer.

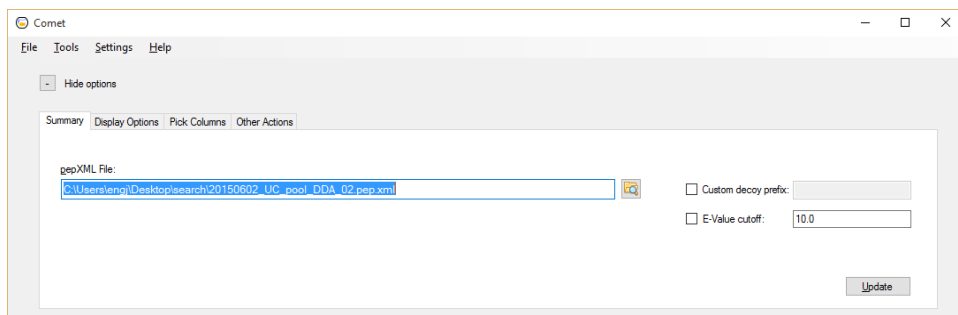
Note that results from a Comet search run via the CometUI will load automatically once the search completes successfully, provided a “*pep.xml*” file was specified as one of the output formats. (Please see the previous section, “Run Search”, for details on running a Comet search from the UI.)

Users may view a previously generated “*pep.xml*” file by following the steps below:

1. Launch CometUI to open up the main window:



2. In the “**Summary**” tab, click the button with the folder icon next to the “**pepXML File**” edit box to browse to a “*pep.xml*” file you want to open (or simply type in the path to the file):



- If the Comet search was run with a custom decoy prefix (other than what is specified in the “*decoy_prefix*” Comet parameter), check the “**Custom decoy prefix**” checkbox, and specify the decoy prefix string in the text box next to it.

Select the E-Value cutoff checkbox and enter a cutoff value to apply an expectation value filter to the results.

☒ Custom decoy prefix:

☒ E-Value cutoff:

- Click on the “**Update**” button , and the results should appear in a list right below the “**Summary**” tab as follows:

pepXML File:
C:\Users\engi\Desktop\search\20150602_UC_pool_DDA_02.pep.xml

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

Displaying 82395 of 82395 total spectra.

☐ Custom decoy prefix:

☒ E-Value cutoff:

Update

SPECTRUM	SSCAN	EXPECT	IONS	PEPTIDE	PROTEIN	CALC_MASS
20150602_UC_pool_DDA_02.00070.00070.2	70	3.04	3/16	R.VAKLFRLAR.L	sp Q969K4 ABT81_HUMAN	1072.686933
20150602_UC_pool_DDA_02.00071.00071.2	71	6.77	3/18	K.LYQHSQQPGK.A	tr C9JD84 C9JD84_HUMAN	1184.593821
20150602_UC_pool_DDA_02.00072.00072.2	72	4.2	4/16	R.RRVFQALAR.I	sp Q6ZUG5 YCO06_HUMAN	1115.667595
20150602_UC_pool_DDA_02.00073.00073.2	73	2.13	5/18	K.QGDKALDFM147.04R.H	sp Q9H987 SYP2L_HUMAN	1193.622664
20150602_UC_pool_DDA_02.00074.00074.2	74	644	3/84	K.KKVASALGICIAIGVGGVLR.I	sp Q6P7N7 TM81_HUMAN	2076.31468
20150602_UC_pool_DDA_02.00074.00074.2	74	32.4	2/20	K.AEC160.03WSQKM147.04SNK.Q	tr H7CS83 H7CS83_HUMAN	1383.591106
20150602_UC_pool_DDA_02.00077.00077.2	77	12.9	1/16	R.LKPAKIDHK.Q	sp Q6WR10 TCS10_HUMAN	1048.639314
20150602_UC_pool_DDA_02.00078.00078.2	78	7.38	4/44	R.TVLDPNSDSNER.V	tr C9JKN6 C9JKN6_HUMAN	1395.626637
20150602_UC_pool_DDA_02.00080.00080.2	80	4.57	9/40	K.SHDVPSKEER.K	sp Q5H9K5 ZMAT1_HUMAN	1311.605508
20150602_UC_pool_DDA_02.00081.00081.2	81	3.54	4/22	K.GPDGYDPQFITK.L	tr Q5JR04 Q5JR04_HUMAN	1336.629932
20150602_UC_pool_DDA_02.00083.00083.2	83	77.9	8/40	R.ATC160.03QM147.04EEQFR.S	sp Q81ZD9 DOCK3_HUMAN	1372.538736
20150602_UC_pool_DDA_02.00085.00085.2	85	15.4	2/18	R.DLLIGDIHGR.S	tr E9PC35 E9PC35_HUMAN	1107.603657
20150602_UC_pool_DDA_02.00088.00088.2	88	1.97	4/20	R.RAQSVSLC160.03C160.03K.A	sp Q75339 CILP1_HUMAN	1264.601626
20150602_UC_pool_DDA_02.00090.00090.2	90	12.8	3/84	R.WFRFC160.03PGC160.03PQALSHDSDHFHER.H	tr E7ET85 E7ET85_HUMAN	2739.181922
20150602_UC_pool_DDA_02.00091.00091.2	91	5.19	5/22	K.WM147.04FPDASEVGSK.K	tr Q5XKG6 Q5XKG6_HUMAN	1281.591089
20150602_UC_pool_DDA_02.00092.00092.2	92	27.4	3/68	K.SETFRLLHAKNIEIRPLK.F	sp Q05780 EXOSK_HUMAN	2163.264042
20150602_UC_pool_DDA_02.00092.00092.2	92	610	1/20	R.C160.03LC160.03SDM147.04DLC160.03K.T	tr I3L141 I3L141_HUMAN	1444.545478
20150602_UC_pool_DDA_02.00117.00117.2	117	1.59	4/64	R.WLC160.03TGDI GEFEPDGC160.03LK.I	tr H7BY27 H7BY27_HUMAN	1995.87065
20150602_UC_pool_DDA_02.00117.00117.2	117	3.64	2/20	K.CETC160.03PROQVDR.L	sp A6NLX4 TM210_HUMAN	1330.604797
20150602_UC_pool_DDA_02.00120.00120.2	120	7.43	5/124	R.KPPMLQPLALPPGLSVHQAERLRLPAVASK.R	sp D15067 PUR4_HUMAN	3426.006107
20150602_UC_pool_DDA_02.00120.00120.2	120	5.92	4/42	-.M147.04ALTPLLLSAGMTLCSPRK.G	tr E7EN07 E7EN07_HUMAN	2283.269431

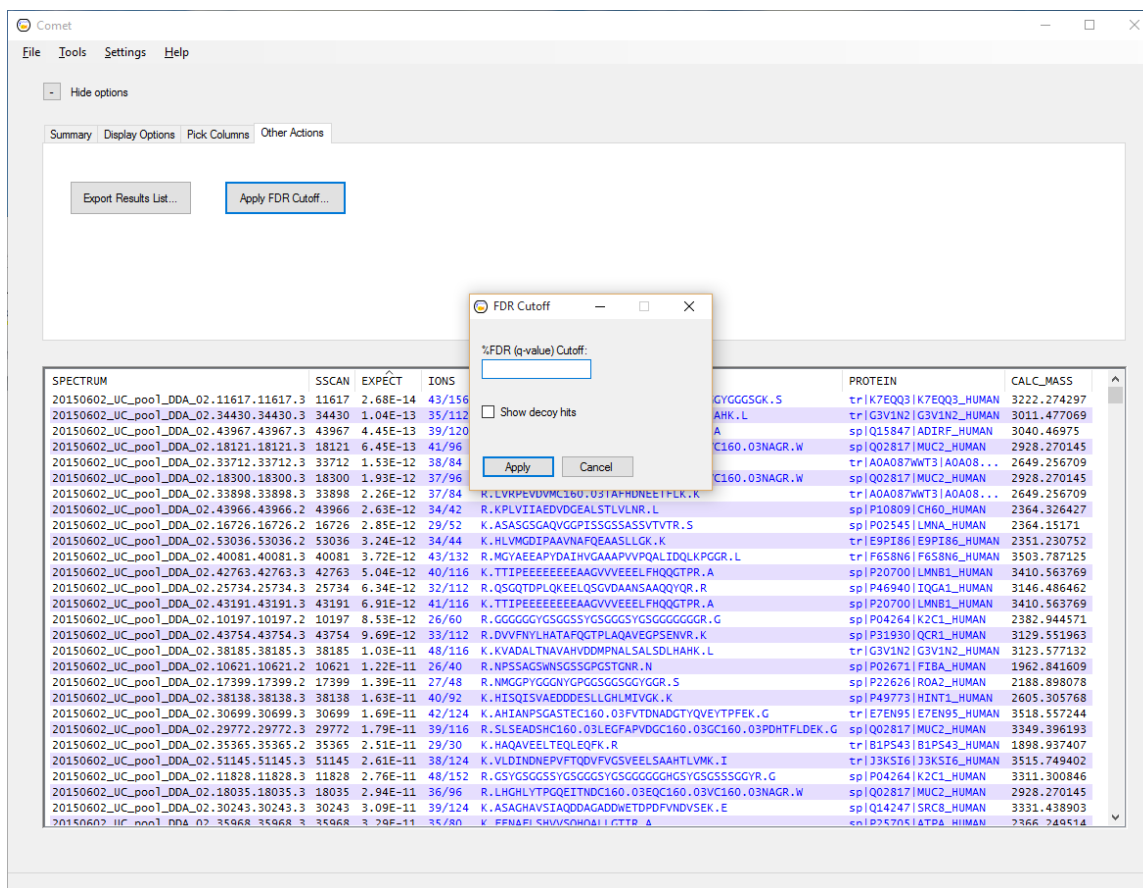
- A summary of information about the results will appear right below the “pepXML File” edit box:

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

Displaying 1996 of 1996 total spectra.

From here on, users can interact with the search results list in several ways, such as clicking on the column headers to sort the list by any of the columns, or clicking on a value in an interactive column with hyperlinks in it (e.g. **Ions**, **Peptide** and **Protein** columns). Users can also manipulate the list by using options available in the “**Display Options**”, “**Pick Columns**” and “**Other Actions**” tabs.

If the search results were from a target-decoy search, a false discovery rate (FDR) analysis can be performed at the PSM level. Click on the “Other Actions” tab and “Apply FDR Cutoff” button to bring up the FDR cutoff dialogue. Specify the FDR cutoff, e.g. enter “5” for a 5% cutoff then hit the “Apply” button. This will filter the identifications at that FDR cutoff. To include the decoy hits in the list, select the “Show decoy hits” checkbox.



The links in the “IONS” column will display the MS/MS spectrum. The links in the “PEPTIDE” column will paste that peptide into an NCBI BLAST page in your browser. Finally, the links in the “PROTEIN” column will display the protein sequence with the identified peptide highlighted.

