VIPER Tutorial

To change look of presentation, run either macro Make_Printable2 or macro Make_OnScreen2

For most useful form when printing, print as "Note Pages"

(If macros are not available, go to "Tools", "Macros", "Security", "Security Levels" tab and set security to Medium. Then close and reopen this file.)

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7/22/2003 version 3.20

Database Analysis Loading – Page 1 "File" menu, "New Analysis (Choose from DMS)"

Select database to analysis from (and export results to).

Shows info about current database.

Buttons that have r function until a .PEI file is selected.

load			Allows us
	Organism Mass Tag Database/Process Type		exact cor
	Organism Mass Tag Database	Configure DB	
	Production Database for Shewanella using "SO" ORFs		Brings up selection
		Select Lockers Select Mass Tags	Brings up selection slide)
no K			
	Database: MT_Shewanella_P45 initialized!		Advand
			loading
US.	Completes loading (since no been selected yet, selecting	D.PEK file ha	S

er to change nection details.

lockers form.

mass tag form (see next

ces analysis to page.

Database stat same as choosing cancel.)

7/22/2003 version 3.20

Database Analysis Loading – Page 1 "File" menu, "New Analysis (Choose from DMS)"

To confine mass tags to only certain types, check one or more of these boxes.

Select mass tag characteristics and push "Include" to include it as a parameter.

	🛚 Mass Tags Selection 🛛 🛛 🔀
	Confirmed mass tags Use subset
7	C Accurate mass tags
	🗖 Lockers mass tags
	Use all mass tags (belonging to MT subset)
	Minimum high normalized XCorr (0 to load all mass tags, regardless of score):
	Dynamic Modifications Inclusion List Del. Clear Is Is Not Any Dynamic none Dynamic none none Image: State of the state of
	AND <u>QR</u> <u>Include</u> > Static Modifications • Is <u>Not</u> <u>Any</u>
	none Cancel DK

Check the "Use subset" box and select a subset of mass tags to use. (Choose All to use from all mass tags in database.)

Inclusion list shows what parameters are used for mass tags loading. (Using more than 1 can sometimes cause odd results.)

7/22/2003 version 3.20

Database Analysis Loading – Page 2

"File" menu, "New Analysis (Choose from DMS)"

Displays info about selected analysis

Displays list of all analyses in database.

Search for analyses containing the search text.

ř	3					Z
	- Selection of ICR-2LS Analysis Resul	File				_
	Dataset/Analysis Folder:	Select	Show <u>A</u> ll	Show Ne <u>w</u>	<u>P</u> rint List	
	012003_SHEW190_Pluto_Sys2C	ol2_1.5ug\ICR	200301221654_/	Auto24026		
	012203_SHEW190_Pluto_Sys2C 012303_SHEW190_Pluto_Sys2C	ol2_0.75ug_ru ol1_0.75ug_ru	12\ICR20030124 13\ICR20030125	1405_Auto2411 0800_Auto2418	7	
	kt20030124_shew190\ICR20030	1301751_Auto	24424		~	
	kt20030120_shew190\ICR20030 kt20030124_shew190\ICR20030	4171014_Auto 4170934_Auto	26894 26898			
	-	_				
	`					
	Creat (m. Chau100		- Search			
	Search for: Jonew 130			rear:		
	<u>D</u> ataset <u>A</u> nalysis <u>E</u> x	periment	↓	<u>P</u> revious	<u>N</u> ext	
			SANET Info	Cancel	ΟΚ	K
	<u></u>					
	Database: MT_Shewanella_P45 initial	ized!				
	Mass Tags Access	\times	Mass Tags	Access		×
	Job=7781		Job=7781			
	NET_TICFit=0.6886296868324	128 225 02	GANET_F	it=1.282737466 lope=4.483879	73086E <mark>-02</mark> 4641612E-03	2
	NET_Intercept=2.3148147738	5387E-04	GANET_Ir	tercept=0.0440	36403699448	8
				·····		
	(OK)			<u> </u>		

Displays GANET information currently in database.

Displays TIC NET information currently in database.

Advances analysis loading to third page.

Completes loading (will not load unless file is selected on page 3).

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Database Analysis Loading – Page 3

"File" menu, "New Analysis (Choose from DMS)"

Selects type of files to display.

Shows files in analysis directory with correct file type.

Opens DMS pages for currently selected ICR-2LS analysis (currently doesn't work).

· · · · · · · · · · · · · · · · · · ·						
Selection of Analysis Result File						
List files of type:						
, <u>,</u>						
94T_062303_withCalibrationandCalLock.PAR						
FTICRDefSettings.txt						
Shew217-5_100uly03_Griffin_0306-5_7_12_2003.PAH Shew217-5_10July03_Griffin_0306-5_7_12_2003.Pek						
Shew217-5 10July03 Griffin 0306-5 7 12 2003 ic.pek						
Date 7/13/2003 1:52:06 PM						
ProcessorLusitania-02-2 Tool ICR2LS						
Priority 2 Dataset Name Shew217-5 10Julv03 Griffin 0306-5						
Dataset Folder Name Shew217-5_10July03_Griffin_0306-5	<u> </u>					
<u>Dataset</u> <u>Analysis</u> <u>Experiment</u> <u>Previous</u>	Next					
IIC Fit Info GANET Info Cancel	ок					
Database: MT_Shewanella_P45 initialized!	· · · ·					
Displays TIC NET and GANET for						
Displays TIC NET AND GAINET TO						

Displays contents of text file (drag and drop a file from the upper list to see it in this one).

Advances analysis loading to fourth page.

Completes loading (with default parameters shown on next page).

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Database Analysis Loading – Page 4 "File" menu, "New Analysis (Choose from DMS)"

Selects type of analysis to be done.

Sets various parameters for file analysis.

Opens DMS pages for currently selected analysis (currently doesn't work.)

Displays TIC NET and GANET for currently selected analysis.

R			
Analysis Parameters —			
Analusis tune:	Standard Individual	_	
	1		leset
Standard MMA=1			
Standard ET=0.2			
Standard ET Type=U Standard UMC=12.5:	2·3·80 Intensity		
UMC Mass=Class Re	presentative		
UMC Abundance=Av	9		
PEK=PEK Pairs N14/N15 Use I	IMC=1		
Pairs N14/N15 MMA	=25		
Pairs N14/N15 ET =0	.15		
Pairs N14/N15 Delta	/pe=0 Mono=0.997		
Pairs N14/N15 Delta	Tol=0.02		
Pairs N14/N15 Use N Pairs ICAT Use LIMC	N Count=1 =1		
I aistext oscome	-1		
<u>D</u> ataset <u>A</u> nal	ysis <u>E</u> xperiment	Previous	Next
	IIC Fit Info	nfo <u>C</u> ancel	<u>0</u> K
Database: MT_Deinococ	cus_P20 initialized!		

-Resets parameters.

This information is stored to the database when exporting, but does not have to be defined.

Completes selection of analysis to load.



Database Analysis Loading "File" menu, "New Analysis (Choose from DMS)"



Auto-analysis is an advanced feature that allows you to process the data for a single analysis using the settings in a .Ini file. You can define the settings to use using File->Save/Load/Edit Analysis Settings. For manual analysis, simply choose "No".

🖶 VIPER	
<u>File</u> <u>T</u> ools <u>H</u> elp	
New	Ctrl+N
New Analysis (Choose from DMS)	Ctrl+Y
New Automatic Analysis (Choose manually)	Ctrl+A
<u>O</u> pen	Ctrl+O
Save/Load/Edit Analysis Settings	
E <u>x</u> it	



Database Analysis Loading "File" menu, "New Analysis (Choose from DMS)"



Loads analysis with all data.

After choosing the file to load, you will be asked if you would like to filter by isotopic fit. This is useful when loading large data files (> 5 Mb) and you plan on filtering by isotopic fit later on. Suggested filter values are 0.15 or 0.20 Alternatively, choose No to load all of the data; you may optionally filter by isotopic fit later on using the Filter form.

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Manually Load PEK file

File menu, "New"

This is necessary if you want to look at the results of an experiment before they are incorporated into the database. To manually load a .PEK file from your computer, go to the File menu, "New". Select the .PEK file from your computer or from a network share and choose OK. Generally, one should choose the calibrated _ic.PEK file or the calibrated _s.PEK file. See the previous two slides concerning the two Yes/No boxes that appear when manually loading a .PEK file.



"Steps" Menu Provides Guide

After loading the PEK file the "Steps" Menu will appear.

This menu guides one through the various steps required to match peaks to mass tags.



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Step 1b. Filter Points

"Steps" menu, "Filter Points"

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<u>Eile S</u>	teps	<u>E</u> dit	<u>I</u> nfo	<u>V</u> iew	<u>T</u> ools	<u>S</u> pecia	al <u>W</u> i	ndow)			
🗃 🗅		9 P	1 🌌	+ +	• •	→ → •	• •	File Nu	m/z MW	Intensity	Expr. Ratio	UMC 'dex
🔁 Uni	titled:	1							966.4500 2,896.32	2720000	149,381.30	
: 151 21 0	MW(Linear or	ale)			Charg	ge State 🗢 🗢	Isotopic	-				
.,									ta Filter			
1,1 # 54:	-								Televenees I Identity and	Comparative Disals		
									ass Bange Charge and	Abundance		
6,00.189	1											
\$ / 4 .015									– Molecular Mass Hange (n Use only Charge Sta	nonoisotopic mass) ate May	600.00	
								-	data with molecular	mass Min	400.00	
4,02,050	{							-	Use only isotopic da	ivini ata Marri	400.00	
						1. Sec.	•	j se de	with molecular mass	within	6000.00	
5,565 2524	1							here the	Tange	Min Chasa Chata and L	400.00	
: 5:4.44										unarge state and is	sotopic uata	
				تقذير					– M/Z Range (isotopic data	a only)		┐
1,485,5161									🔽 Use only Isotopic da	_{ata} Max	2000.00	
								1999 - 1999 1997 - 1999 - 1999 - 1999 - 1999 - 1999 - 1999 - 1999 - 1999 - 1999 - 1999 - 1999 - 1999 - 1999 - 1999 - 1999 -	with m/z within rang	le Min	400.00	
44.142	1	A: 94	1,414	1,005 2,05	a 2,21	2,292 2,169	4,24	4,in 5,#2				_
1												
									00.0% visible (99,259 out of	99,289 data point:	s)	
									Reset to Apply	Use	<u>о</u> к	<u>C</u> ancel
									None <u>N</u> ow	Defaults		

Coordinates display ("View" menu, "Coordinates") – Displays coordinate information when you move your mouse over a data point on the graph.

After searching the database, filter out all data that wasn't identified by selecting "Exclude unidentified data" on the "Identify and Comparative Display" tab.

Set parameters to filter on. Default parameters are:

1.Exclude data with isotopic fit < 0.2.

2.Mass range 400-6000.

3.m/z range 400-2000.

4.Charge state 1-6.

Click "Apply Now" to filter. Click Reset for no filters.

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7/22/2003 version 3.20

Display TIC and BPI Plots

"View" Menu, "TIC and BPI Plots"

Choose between various TIC (total ion chromatogram) plots, or a BPI (base peak ion) plot.

Automatically update plot when checked.



7/22/2003 version 3.20

Step 2. Find Unique Mass Classes

Steps Menu, "Find UMCs"

There are several ways to find the UMCs. The two main options are:

"UMC 2003"

 - "Favor Higher Intensity" is the fastest UMC search method, but creates the lowest quality UMC's.

-"Shrinking Boxes Favor Intensity" is the next slowest UMC search method, and creates better quality UMC's.

"UMC Ion Networks"

– This is the slowest UMC search method, but it creates the highest quality UMC's.



Step 2. Find UMC 2003 (Unique Mass Classes) "Steps" Menu, "Find UMCs", "UMC 2003"

Select whether UMCs are done for all data points in display or only for the current view. (Use of Current View is useful if the user has filtered out data using Filter Points and you only want to search the filtered data.)

Mass Tolerance, total range in UMC can be up to twice this number.

Start finding UMCs using current settings.



Controls function used to produce UMCs. Favor Higher Intensity and Shrinking Box are best.

Definition of class abundance

Definition of class MW.

Controls what type of gaps (scans in which no member of the UMC is found) are allowed. Normal settings are 10, 3, and 3.

Displays UMCs (and parameters) as a text file. Can be used to save UMCs as a text file.

7/22/2003 version 3.20

Step 2. Find UMC 2003 (Unique Mass Classes) "Steps" Menu, "Find UMCs", "UMC 2003"

Auto-refine options can be used to filter out UMC's that have too few or too many members.

Split UMC's can be used to look for UMC's that contain 2 or more distinct populations of ions, based on abundance.

UΝ	AL Definition Auto Refine U	ptions	
_	Remove low intensity classes	s(%)	30
	Remove high intensity classe	es(%)	30
~	Remove cls. with less than	3	members
~	Remove cls. with more than	150	members
-s	plit UMC's Options		
V	Split UMC's by Examining A	bundan	ce
M in	linimum difference 1 average mass	5	ppm
M C	laximum peak ount to split UMC	4	peaks
P in	eak picking itensity threshold	15	% of max
Ρ	eak picking minimum width	6	scans

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Step 2. Find UMC Ion Networks Use instead of UMC 2003 method. "Steps" menu, "Find UMCs", "UMC Ion Networks"

□ UMC Ion Networks 1. Find Connections 2. Edi Definition Scope C All Data Points C Qurrent View	S WFilter Connections 3. Define UMC's using Connections Metric Type Euclidean Image: Use Monoisotopic Mass Image: Use Monoisotopic Mass Image: Use Monoisotopic Mass Image: Use Average Mass Image: Use Average Mass Image: Use Average Mass Image: Use Log (Abundance) Image: Use SCAN Image: Use Fit Image: Use Image: Use Image: Use Fit Image: Use Image: Use Image: Use	Set to Defaults 0.025 Da	 Select the "All Data Points" or "Current View" option. The default parameters should work fine. Click "Find Connections".
Close Nonet structure The options on Connections (type The parameters UMC 2003 Option Click "Find UMC	Tab 2 can be used to filter the bically skip this). on Tab 3 are similar to the ons. 's" to identify the UMC's.	Works 1. Find Connections 2. Edit UMC From Net Class Representative Highest Abundance Sum of Class Abundance Sum of Class Abu. Class Mass Class Mass Class Median Classes Make single-member Classes No net structure	S Auto-Refine Qptions Split UMC's Options Auto-Refine Options Split UMC's Options Remove low intensity classes(%) 30 Remove high intensity classes(%) 30 Remove cls. with less than 3 members Remove cls. with more than 150 members Find UMC's Herove cls. with more than 150 members Auto-Refine Qption the polate: 3 UMC Draw Type Actual UMC e found!



Display UMCs

"View" Menu, "Unique Mass Classes"



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Zoom in on Single UMC

Use mouse to select rectangular region to expand.



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Step 3. Select Mass Tags (Connect to DB)

This step can be skipped if the data was loaded using the "New Analysis (Choose from DMS)" method to select a datafile.

1 Select the	Select/Modify Database Connec	tion
database.	MT_Shewanella_P45, 110016 mass tags MT_BSA_P47, 133 mass tags MT_Shewanella_X27, 22051 mass tags MT_Yeast_P51, 9048 mass tags	Details for the selected connection in the list at left Database Name: MT_Shewanella_P45 Count of selected mass tags in selected DB: 110016 Mass tag subset ID: AMT's Only Confirmed Only Lockers Only Minimum high normalized XCorr: 0
2.Link to the database.	Sort by Most Recent ■ Link to Selected DB □ Link to DB Not Listed Above □ Break Current DB Link □ Cancel □k Database I Job number PEK Source	the currently connected database Name: MT_Shewanella_P45 elected mass tags in current DB: 125895 <u>Select Mass Tags</u> Dhy Dynamic 1 And Static 1 ed Only s Only gh normalized XCorr (0 to load all mass tags, regardless of score): 2 nfo for the current gel file r: 30909 MD_Type: 1 e File: PMix2_9T_04July03_Griffin_0306-5_7_6_2003.Pek

7/22/2003 version 3.20

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Step 3. Connect to Database: Details

If the datafile was selected using File menu, New, then this step cannot be skipped.

Recently selected databases are shown here (Double-click to connect to it).

Sort database list above by most recent or _____ alphabetically.

Link with selected database from list above.

Link to a database not shown above.

Break the current link to a database (most often used to switch links from one database to another).

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Select/Modify Database 0	Connection	3
MT_Shewanella_P45, 110016 mass tags MT_BSA_P47, 133 mass tags MT_Shewanella_X27, 22051 mass tags MT_Yeast_P51, 9048 mass tags	Details for the selected connection in the list at left Database Name: MT_Shewanella_P45 Count of selected mass tags in selected DB: 110016 Mass tag subset ID: AMT's Only Confirmed Only Lockers Only Minimum high normalized XCorr: 0	Ir se th (s
Sort by Most Recent	Details for the currently connected database Database Name: MT_Shewanella_P45 Count of selected mass tags in current DB: 125895 Mass tag subset ID:	In cu fi (I S ta di sl

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Information on selected database from the list on the left (such as modifications)

Information on the current database the file is connected (linked) to.

Select specific mass tags for the current database (See next slide for more details).

Step 3. Connect to Database: Details

To confine mass tags to only certain types, check one or more of these boxes.

Select mass tag characteristics and click "Include" to include it as a <u>parameter</u>.

)	📓 Mass Tags Sele	ction		
	🔲 Confirmed mass tags	🔲 Use subset		•
of 🗾	🔲 Accurate mass tags			
	🔲 Lockers mass tags			
	🔲 Use all mass tags (belor	nging to MT subs	et)	
	Minimum high normalized X(Corr (0 to load all	mass tags, regardless o	of score): 0
	Dynamic Modifications			
	⊙l <u>s</u> ⊂ls <u>N</u> ot	C <u>A</u> ny In	clusion List <u>D</u> el Junamic none And Stat	. Clear
	none	-		
			'	
	AND OR	I <u>n</u> clude >		
	Static Modifications			
	⊙l <u>s</u> ⊂ls <u>N</u> ot			
	none	-	Canaal	or 1

Check the "Use subset" box and select a subset of mass tags to use. (Choose All to use from all mass tags in database.)

Filter by high normalized XCorr.

Inclusion list shows what parameters are used for mass tags loading. (Using more than 1 can sometimes cause odd results.)

7/22/2003 version 3.20

Function menu – Use to calculate NET and to view and export results as a text file.

Use the lowest percentage of highabundance UMCs (20%) while maintaining the number of IDs (from the iteration box) greater than the minimum matching UMC count.

Controls what MW tolerance is used to identify hits for calculating NET.

NET tolerance for selecting hits to calculate NET.

Define how to ______ iterate the calculations.

Auto-adjust % of high abundance UMC's to use.

Step 4. NET Adjustment

Edit Menu, "Net Adjustment" -> "UMC ID Peaks" When opening, may take a few minutes for mass tags to load.



Mass Tags menu – Use to check the status of mass tags, reload mass tags, or load mass tags from a legacy database.

Elution Formula menu – Use to reset NET Calculation Formula back to Generic.

Define the criteria for selecting peaks when calculating NET.

Results from calculating NET after each iteration.

Reset to Generic NET equation and default start values.

7/22/2003 version 3.20

Step 5. Database Search (for UMC to Mass Tag Identification)

"Steps" menu, "Database Search"

There are several ways to search the Mass Tag database. The two most common options are:

"UMC Single Mass" only uses the median mass of each UMC, and there is just 1 unique mass for the UMC and only one search of the database performed (for each UMC). If a match is found using the median mass, the result is stored in all of the ions for the given UMC. A time value (NET value) is also used for the search.

"UMC Ion-by-Ion" compares the mass of each ion (mass spec peak) in a given UMC with all of the mass tags in memory. If a match is found, then all of the ions in the given UMC are assigned the match. This is best when the UMC's have a large spread in mass, and the median mass may be too far away from the mass in the database. With this method, a UMC with 10 members will have 10 unique masses used for searching the database.



Step 5. Database Search (for UMC to Mass Tag Identification)

"Steps" menu, "Database Search", "UMC Single Mass"



7/22/2003 version 3.20

Step 5. Database Search (for UMC to Mass Tag Identification) "Steps" menu, "Database Search", "UMC Ion-by-Ion"

	Search Mass Tags DB - UMC	
	<u>Function</u> Mass Tags <u>Elution</u> Time	
3. Search All UMCs	MTDB Status: Mass tags count: 127783	a la
	Search All UMC's Image: Dipolate data in current with results of search Molecular Mass Field Molecular Mass Tolerar O Average Tolerance ⊙ gpm	1. Set the Mass
2. Set the NET Tolerance	• Monoisotopic ○ Ihe Most Abundant • Data and and • NET Calculation • O Data and • All results • Eormula • All results • Eormula • First choice • 0.0001172959 * FN + (0.100427459 • Tolerance • 0.05 • Modifications • Alkylation • ICAT d0 • Mass correction:	Tolerance Note: Old matches are automatically removed when a new search is performed.
	UMCs pairing status ET: GANET	

7/22/2003 version 3.20

Step 6. Tolerance Refinement "Steps" menu, "Tolerance Refinement" Improve mass accuracy by comparing the observed Mass Tags Molecular Weight to the value predicted by the database.

This function automatically calculates the histogram of the difference between the observed and predicted molecular weights.

To shift the peak of the histogram to a mass error of zero click "Start Re-calibration".

NOTE: After recalibrating the data search the Mass Tag database again using a more strict mass tolerance.

Tolerance Refinement (Mass and GA	NET Error Plots)	Before the
Eile Edit <u>V</u> iew		rocolibro
Mass Calibration Refinement Tolerance Refinement Tolerance Type © ppm © Dalton Auto recalibrate Manually recalibrate	Mass Error (PPM) Show Tolerance Refinement Controls MTDB Status: Mass tags count: 11388 Data points with 1 or more hits = 23283 Job 30909: PMix2_9T_04July03_Griffin_0306-5_7_6_2003.Pek	peak is u not cente around z
Revert to Original Overall Adjustment -0.7037 ppm New Adjustment (relative to overall) 0 ppm Note: All data is shifted by a constant ppm value, and thus a varying absolute Da value. The ppm shift amount is determined by the location of the peak apex in a ppm-based mass-error plot.	Count 2000 1500	After cal the peak occur at
Criteria To Use Peak For Refinement Minimum Height 100 counts/bin Pct of Max for Finding Width 30 Current DB Search Tolerances DB Mass Tolerance: 25 ppm DB NET Tolerance: 0.1 NET Mass Calibration Plot Status Peak Center: 0.068 ppm Peak Width: 6 ppm Peak Width: 1889 counts/bin Peak Height: 1889 counts/bin	1000 1000 MC's 500 108 ppm 500 500	The widt should b ppm for data and >10 ppn Qstar da

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ne tion the isually ered ero.

bration should zero.

h of this e <10 FTICR may be for ta.

7/22/2003 version 3.20

Step 7. UMC Delta Pairs

"Steps" menu, "Find Pairs" -> "Delta"

Function menu – Use to find pairs, clear pairs, recalculate ER, etc.

Delta MW used to find pairs. (in Daltons)

Max and min deltas to consider for a pair, or automatic calculation (easiest and most accurate thing to do).

Maximum scan difference that can occur between the starting scan of the low UMC and the starting scan of the high UMC.

👶 UMC Delta Pairing Analysis 🛛 🛛 🔀	Report menu –
Function <u>R</u> eport	Use to export
This function works on UMC rather than individual distributions. Abundance of the class is determined from the UMC definition. Expression Ratio calculation is defined with general options. Function always works on current UMCs.	various pairs reports to text files.
Delta: 0.997 Pair Tolerance: 0.02	Allowed difference
Calculate Min/Max Deltas from class molecular mass	between actual
Min Deltas: 1 Max Deltas: 100	and calculated MW of high pair
Scan Tolerance: 3 🔀 Require pair-classes overlap	member (in
ER Inclusion Range: -5 to 5	Require high and
	low pairs to be

found together in

at least one scan.

ER Inclusion Range, used with some of the options in the "Function" menu.

7/22/2003 version 3.20

Step 8. UMC N14/N15 Pairs Identification

"Tools" menu, "Search Mass Tags Database", "UMC N14/N15 Pairs"

Pairs menu – Use to eliminate certain Mass Tags menu – Use to check status of kinds of pairs and export results to MTDB. mass tags or load tags from legacy DB.

Report menu – Use to export various pairs reports to text files.

Shows status of loaded mass tags.

Controls type of mass tag MW used for UMC identification.

Controls which identifications are output for each pair, all or only the best one.



the "Elution Time" menu.)

Elution Time menu – Use to change elution time slope and intercept between Generic, TIC Fit NET and GANET.

Controls mass tolerance for identification

Searches with current settings.

NET type as last selected in "Elution Time" menu.

7/22/2003 version 3.20

"Export Data" function

"Special" menu, "Export Data"

Select from any of your open Gel files to export its data. -

Choose whether to export all data points, or only those currently shown on the 2D -Display (useful if you've filtered points and only want them exported).

Select whether you'd like the NET calculated using Generic, TIC, or GANET.

[🖷 Export Data		×	
	Select display to export			
	C:\Jason\Analyses_DRAD\(3_12_03_DRAD_X26\Job26328.	·	
	Export Scope	Molecular Mass Type C Average Monoisotopic C The most abundant	•	Select which molecular mass type you would like to be used when exporting data.
,	NET Calculation Generic O TIC (FN-MinFN)/(MaxFN-MinFN	C GANET C GANET C UMC		Select whether to export the data points or just the Unique Mass Classes (UMCs).
	C:\Jason\Current_Analysis\E) ataFile.txt	\leftarrow	Export location
	Close	Export Browse] <	Click to choose where you want the data exported to.
	Click t sele	to export data with cted parameters.		

7/22/2003 version 3.20

Report Saving and Excel Import Microsoft Excel, "File" menu, "Open", select a .txt file

Sample Report

🖫 UMC Report
<u>F</u> ile
Generated by: Contemporary 2D Displays - 3.9.5 Unique Mass Classes(UMC) on all data points! UMC type: Intensity with shrinking box, Averagi Intensity
Nolecular mass: Monoisotopic Class abundance: Average of member abundances Class molecular mass: Mass of class representat Molecular mass tolerance: 12 Snum
Number of allowed gaps: 2 Allowed size of gap: 3 Allowed percentage of gaps: 80.00%
UMC_ID;UMC_Cnt;UMC_Rep_MW;Scanl;Scan2;UMC_Avg_F
File menu – Use to save
file, print, or close window

Report data.

Sets delimiter(s) used for moort.

The Text wizard has determin	ed that your data is Delimit	ed.		
Original data type	or choose the data type tr	hat best describes your dat	.a.	(del
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Sets style of import file (delimited or fixed width.)

Advance import to second page

7/22/2003 version 3.20

Copy Points (UMCs) in View to Clipboard Function

"Edit" menu, "Copy Points in View to Clipboard"

This function copies the Scan Number, GANET, UMC Index, Abundance, Charge state, m/z, monoisotopic mass, and any database match information for all of the data currently "in view" to the clipboard. Thus, if you zoom into a narrow region showing 10 spots, you can use this function to copy that data, where you can then open MS Excel and paste it in there.

<u>Note</u>: When "Include Empty Scans when Copying" is true, then empty lines are included in the copied list for scans with no ions. This can make it easier to line up the data between various analyses, or between different mass regions, but covering the same scan range.

"Edit" menu, "Copy UMCs in View to Clipboard"

This function copies the UMC index, ScanStart, ScanEnd, Average GANET, UMC monoisotopic MW (median of all UMC points), UMC MW standard deviation, UMC abundance, Range of charge states, Number of points in UMC, UMC average fit, Expression ratio, Number of mass tags the UMC matched, Mass Tag ID, Mass Tag monoisotopic MW, Mass Tag modifications, Number of points in UMC matching the Mass Tag of the UMCs currently "in view" to the clipboard.

