

User Interface

The screenshot shows the CCMS user interface with a blue header bar. The header includes the CCMS logo, the text "Computer Science and Engineering University of California, San Diego", the "Center for Computational Mass Spectrometry" name, and a "BETA" indicator. Below the header is a navigation menu with links: Logout, Update Profile, Jobs, General Info, UCSD Proteomics, Future Tools, Demo, and Contact.

Workflow Selection

Workflow: NAP_CCMS

Title: nap_interface_test

File Selection

GNPS job ID: ce2a564dbd

Number of a cluster node: 40

N first candidates for consensus score: 10

Accuracy for exact mass candidate search.: 10

Acquisition mode: Positive

Multiple adduct types: [empty input]

Structure databases: DNP,SUPNAT

User provided database: Select Input Files

User provided MetFrag parameter file: Select Input Files selected

Maximum number of candidates structures in the graph: 10

Workflow Submission

Input one or more databases, separated by ",".
Available options are:GNPS, HMDB, SUPNAT, DNP, CHEBI. Use none to select only user defined.

1 file and 0 folders are selected

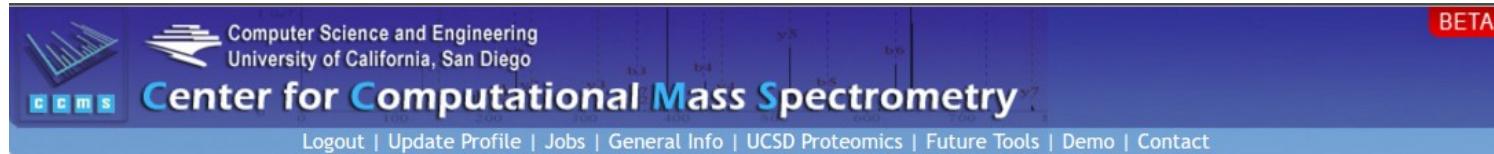
Whether to use the *fusion* ranking to select the *n* first candidates of neighbors
Cosine value to subselect inside a cluster: 0.5
 Use fusion result for consensus

Adduct ion type: [M+Na]

Compound class to be selected: [empty input]
 Skip parent mass selection

ClassyFire class in the following format: "class:name"
Example:
superclass_name:Benzenoids

User Interface



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Acquisition mode: Positive

Multiple adduct types:

Structure databases: DNP,SUPNAT

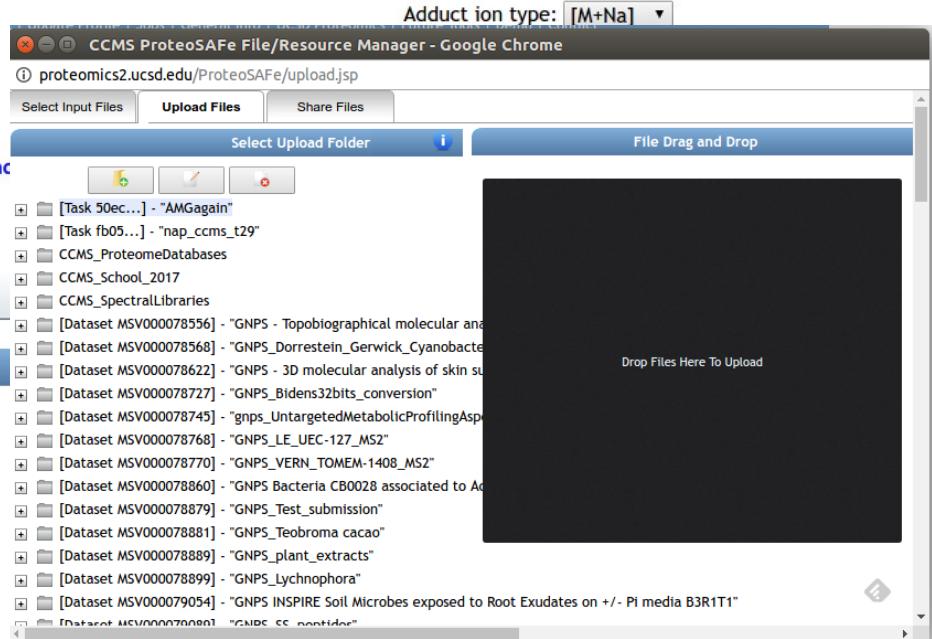
User provided database: Select Input Files

User provided MetFrag parameter file: Select Input Files selected

Maximum number of candidates structures in the graph: 10

Workflow Submission

To use an user provided structure database select the Drag and Drop upload menu and upload the tsv file formated as describe in tooltip (?)
The user database can be used in addition to default databases or used individually setting *Structure databases* parameter to “none”



Workflow monitor

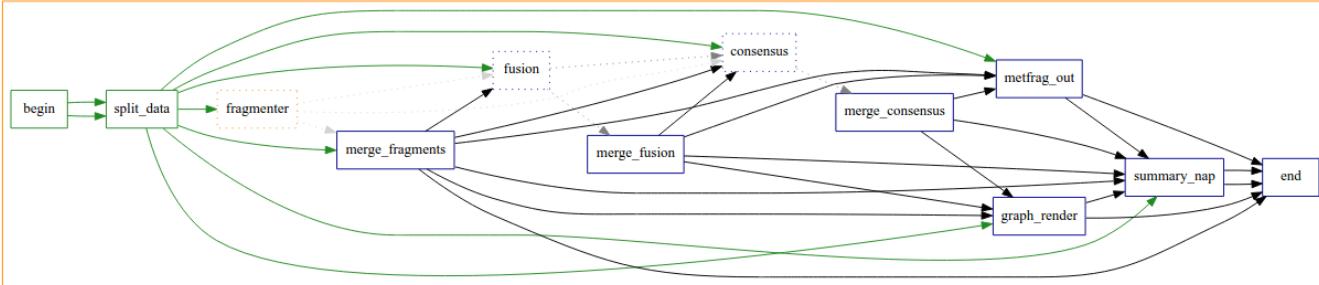
Computer Science and Engineering
University of California, San Diego

BET

Center for Computational Mass Spectrometry

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Job Status	
Workflow	NAP_CCMS2
Status	RUNNING [Clone] [Delete]
User	rsilva (ridasilva@ucsd.edu), University of California, San Diego
Title	nap_interface_test
Date Created	2017-08-24 13:57:04.0
Execution Time	2 minutes 2 seconds
Progress	

Results Page

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University of California, San Diego
Center for Computational Mass Spectrometry

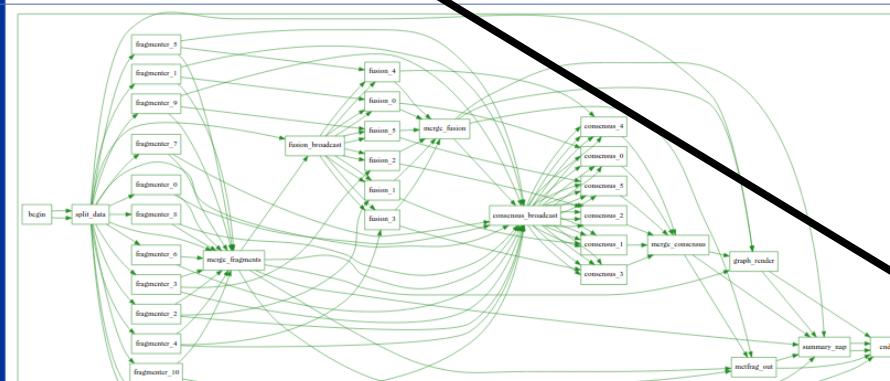
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Job Status

Workflow	NAP_CCMS
Status	DONE [Clone] [Summary Report]
User	rsliva (ridasilva@ucsd.edu) University of California, San Diego
Title	nap_interface_test
Re-Analyze Task Outputs	Import to Re-analyze Task Data
Date Created	2017-08-17 11:47:27.0
Execution Time	8 minutes 43 seconds

Progress



[Restart][Delete]

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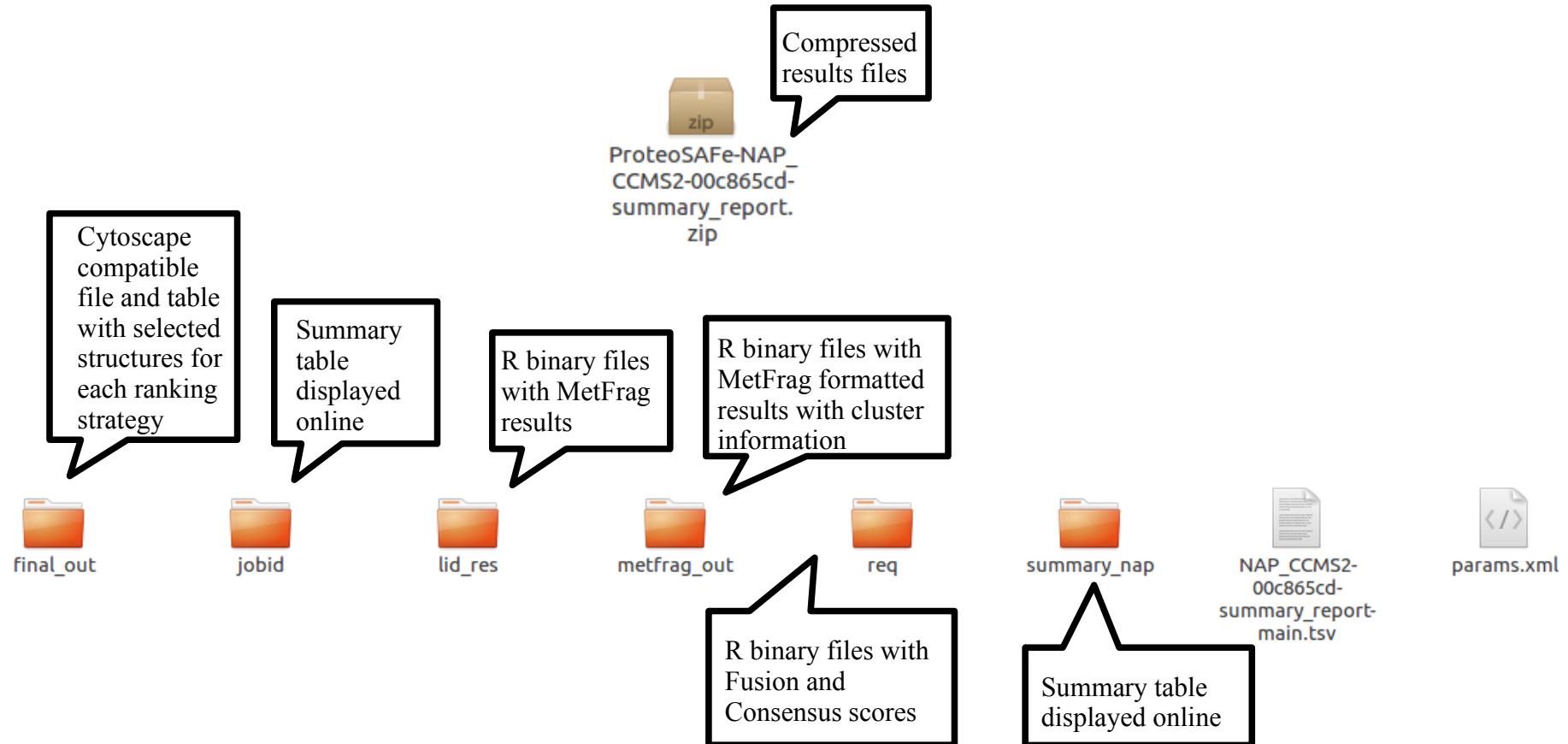
Download Option: Tab-Delimited Result Only
Include Entries: Filtered All [Download](#)

Summary table with the results of IDs and Class of compounds inside the group of the first ranking structure by each scoring strategy

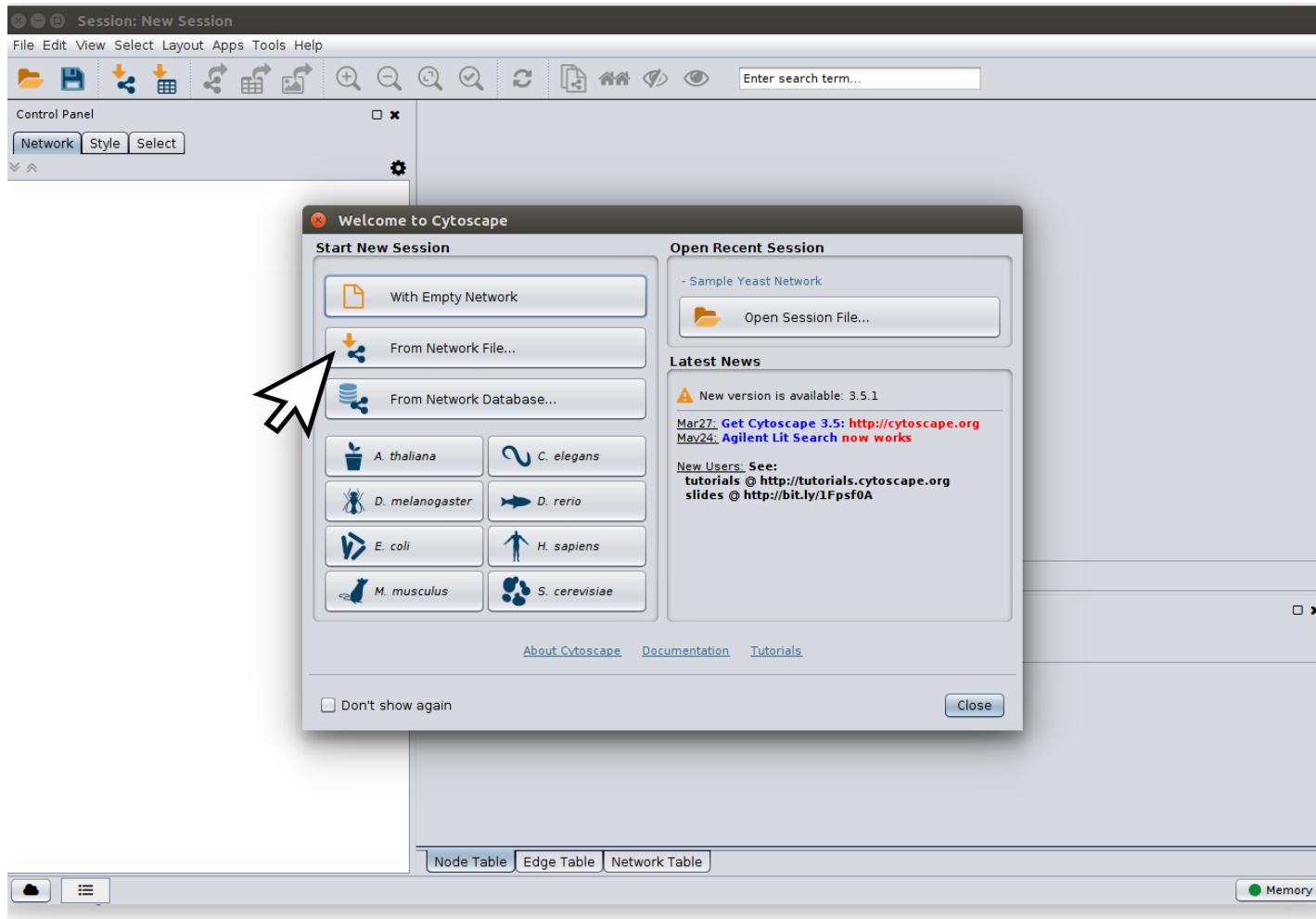
nap_interface_test						Hits 1 - 6 out of 6	Go to	Go
Select columns						MetFragID	MetFragSC	
Filter	cluster.index	Parent Mass	RT	LibraryID	MetFragID	MetFragSC		
1	34	827.339	907.145	euphorboidinT	SN00004286#SN00023815#SN00025151#SN00132116#CCMSLIB00000578251#SN00061408	Organoheterocyclic compounds#Organic acids and derivatives#NA		
2	40	841.353	1069.950	N/A	QMT68#SN00245602#CFG34#SN00247561#PKG63#SN00353054#LGT03#SN00064161#SN00275612#SN00298127#SN00253343#CDP26	Organoheterocyclic compounds#Alkaloids and derivatives#Organic acids and derivatives		
3	46	861.320	975.383	N/A	GQX73#SN00024393#SN00139900#SN00070780#SN00074249#QXM36#SN00098223	Alkaloids and derivatives#Organoheterocyclic compounds#Organic acids and derivatives#Organic oxygen compounds		
4	426	785.325	645.822	N/A				
5	453	799.339	809.114	N/A				
6	549	861.322	978.120	N/A				

Download Results

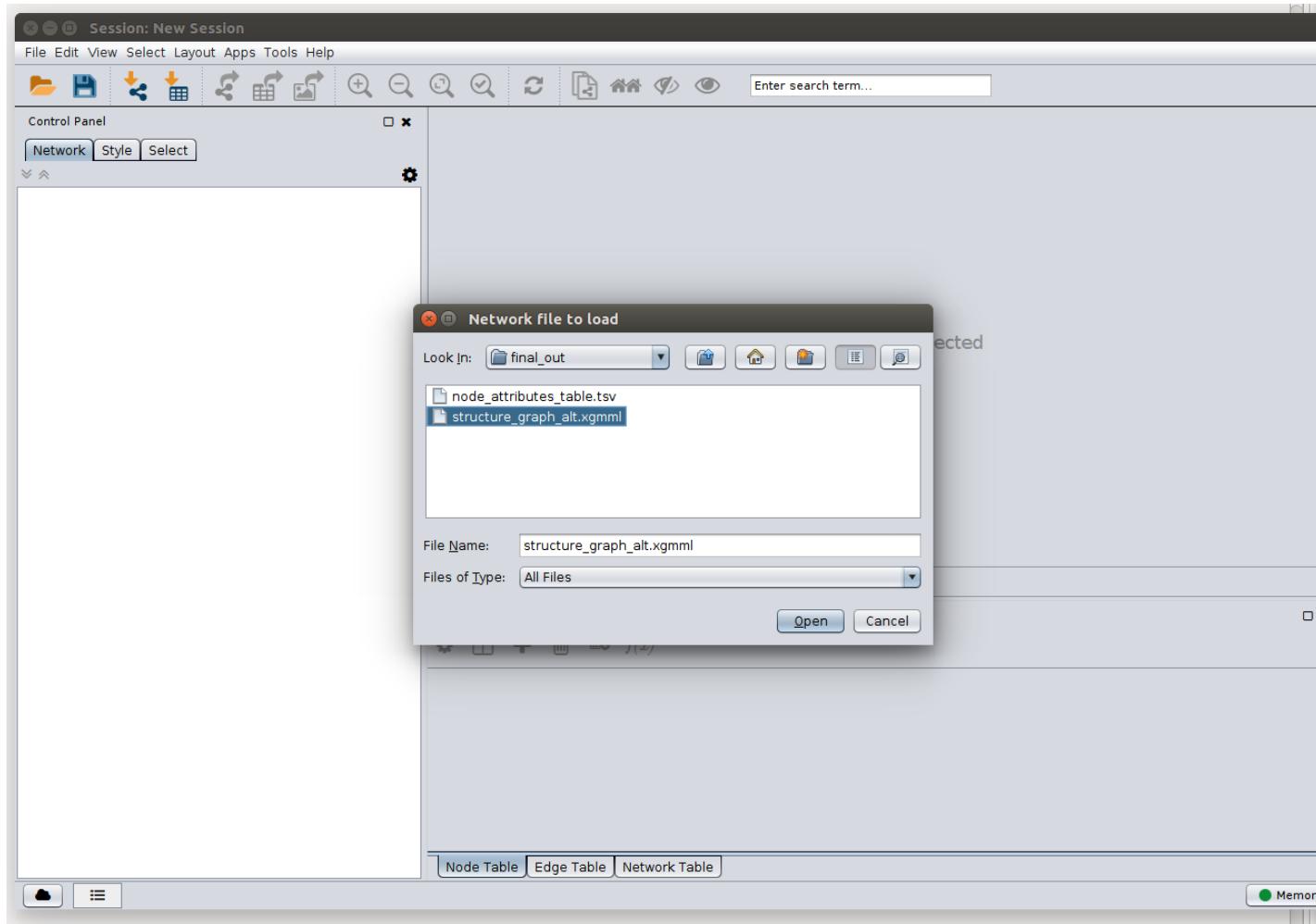
Result Files



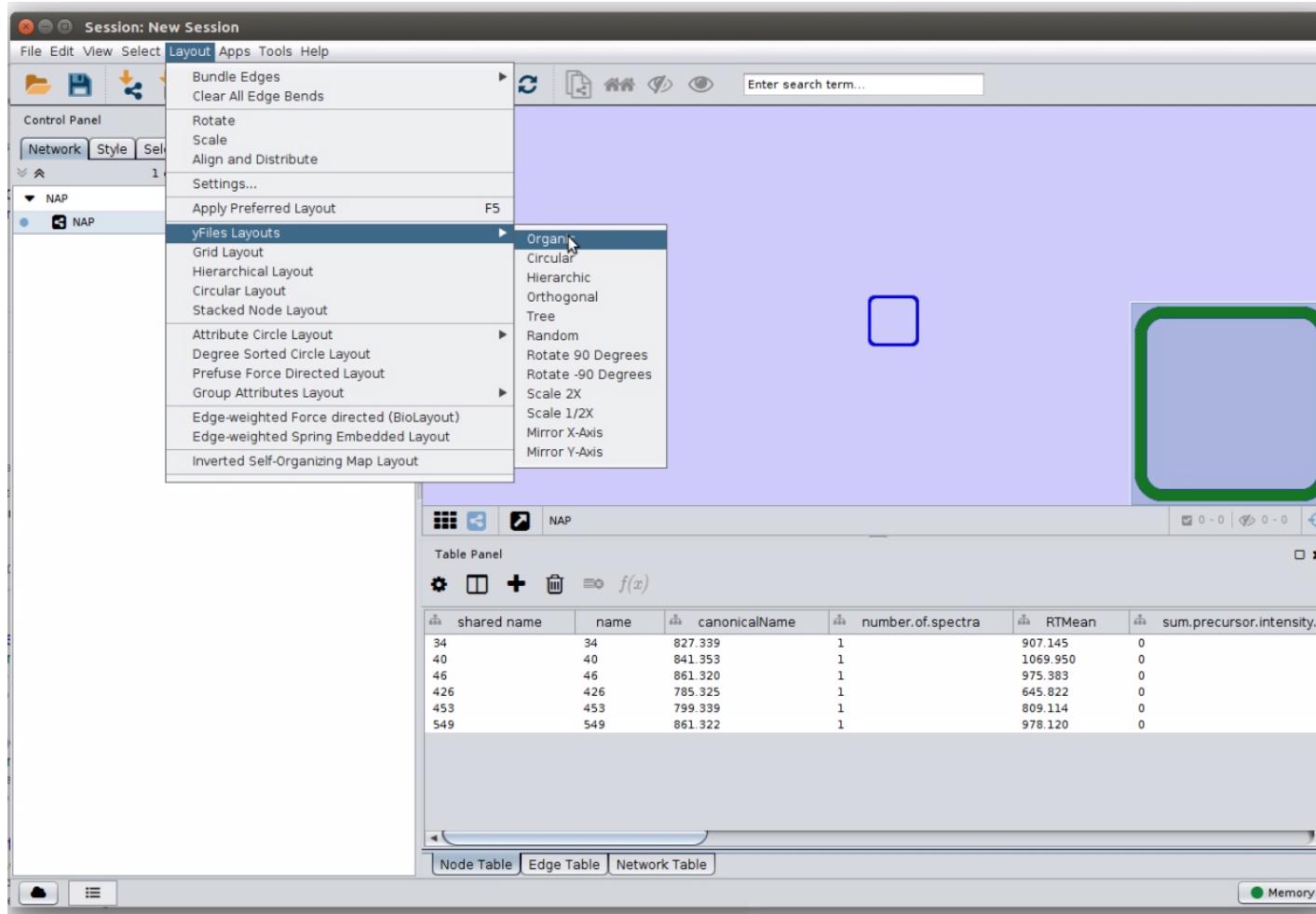
Use Cytoscape From Network File import function



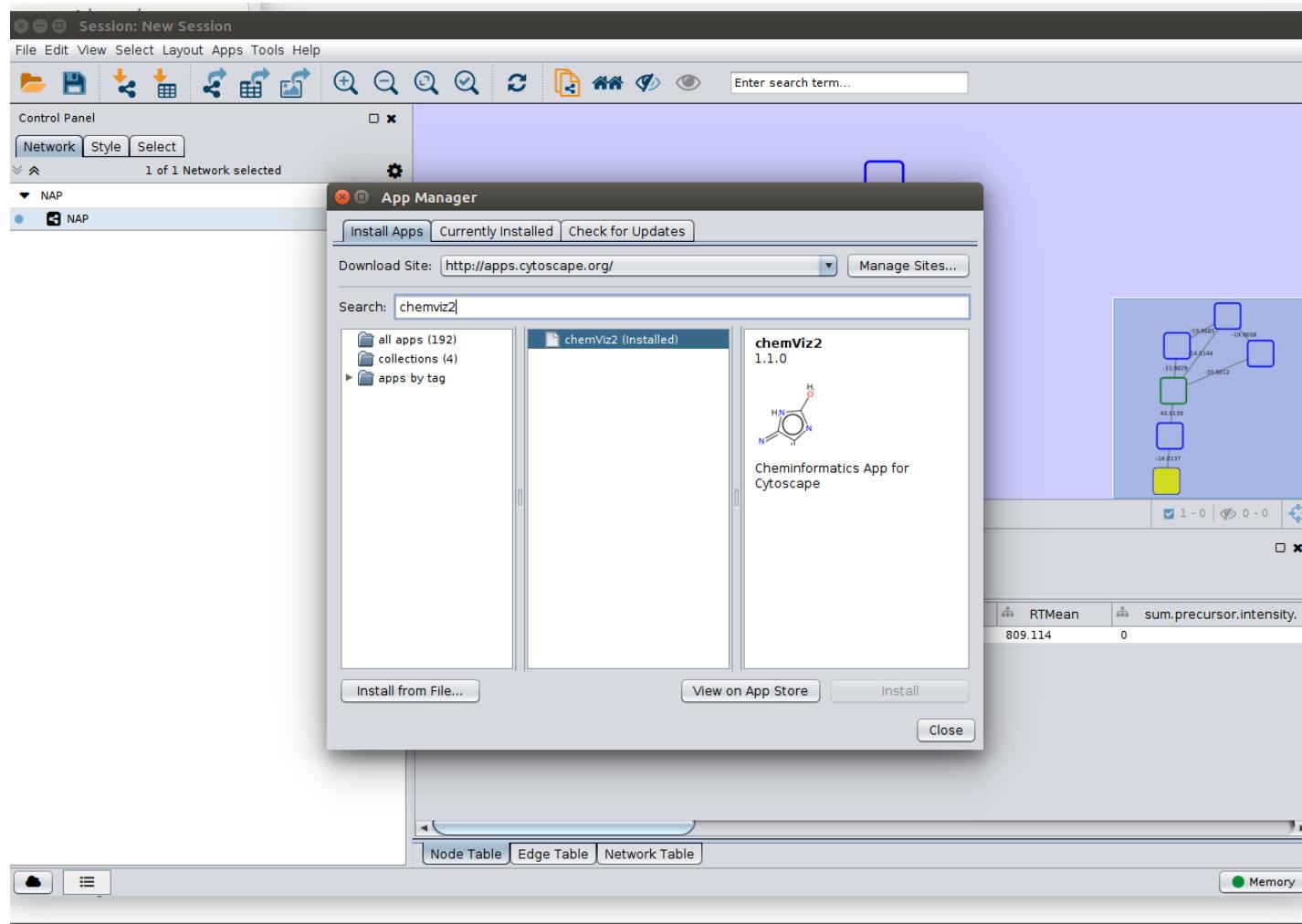
Import the file *structure_graph_alt.xgmm* inside *final_out* folder



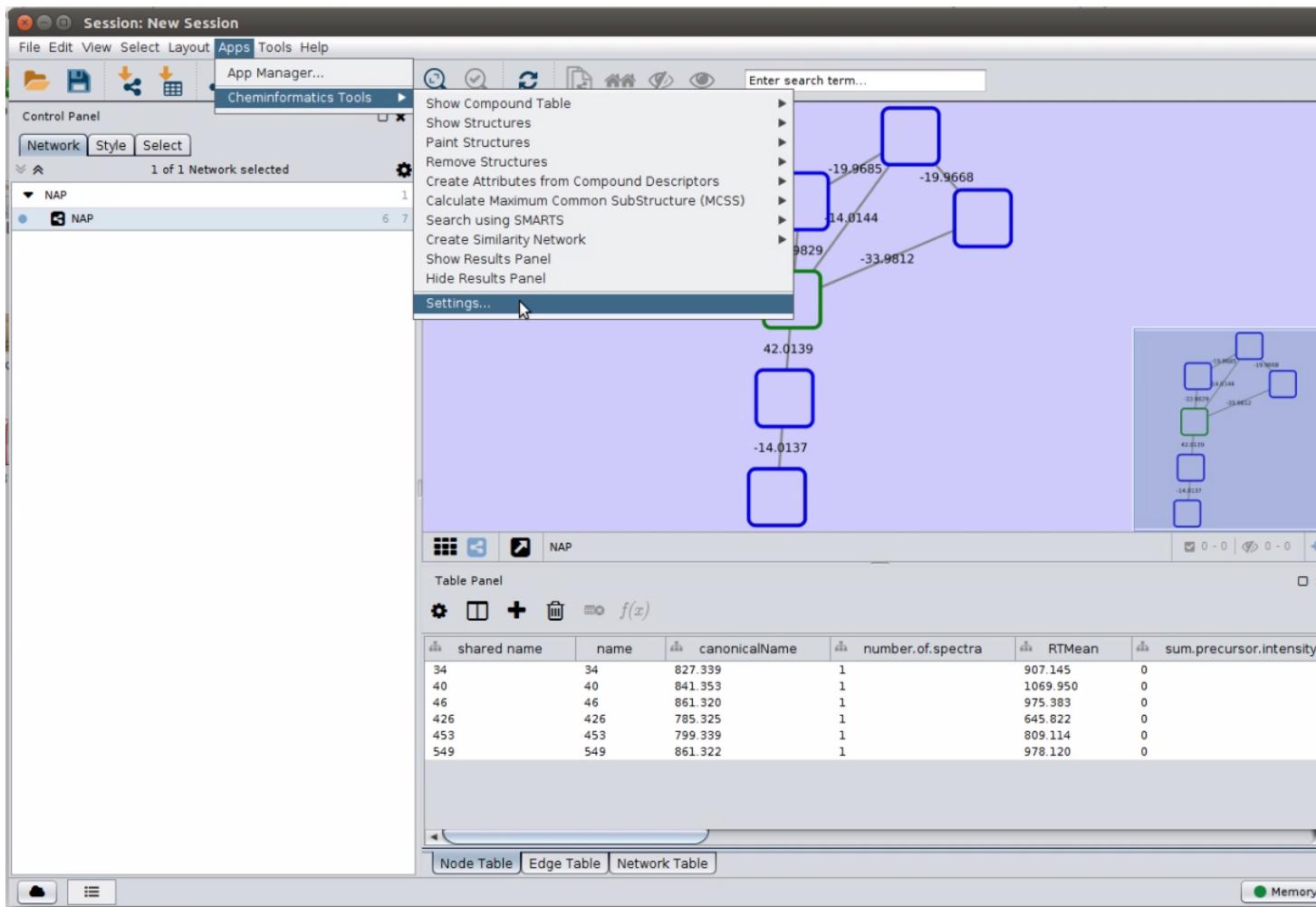
Apply a layout to spread the nodes and help visualization



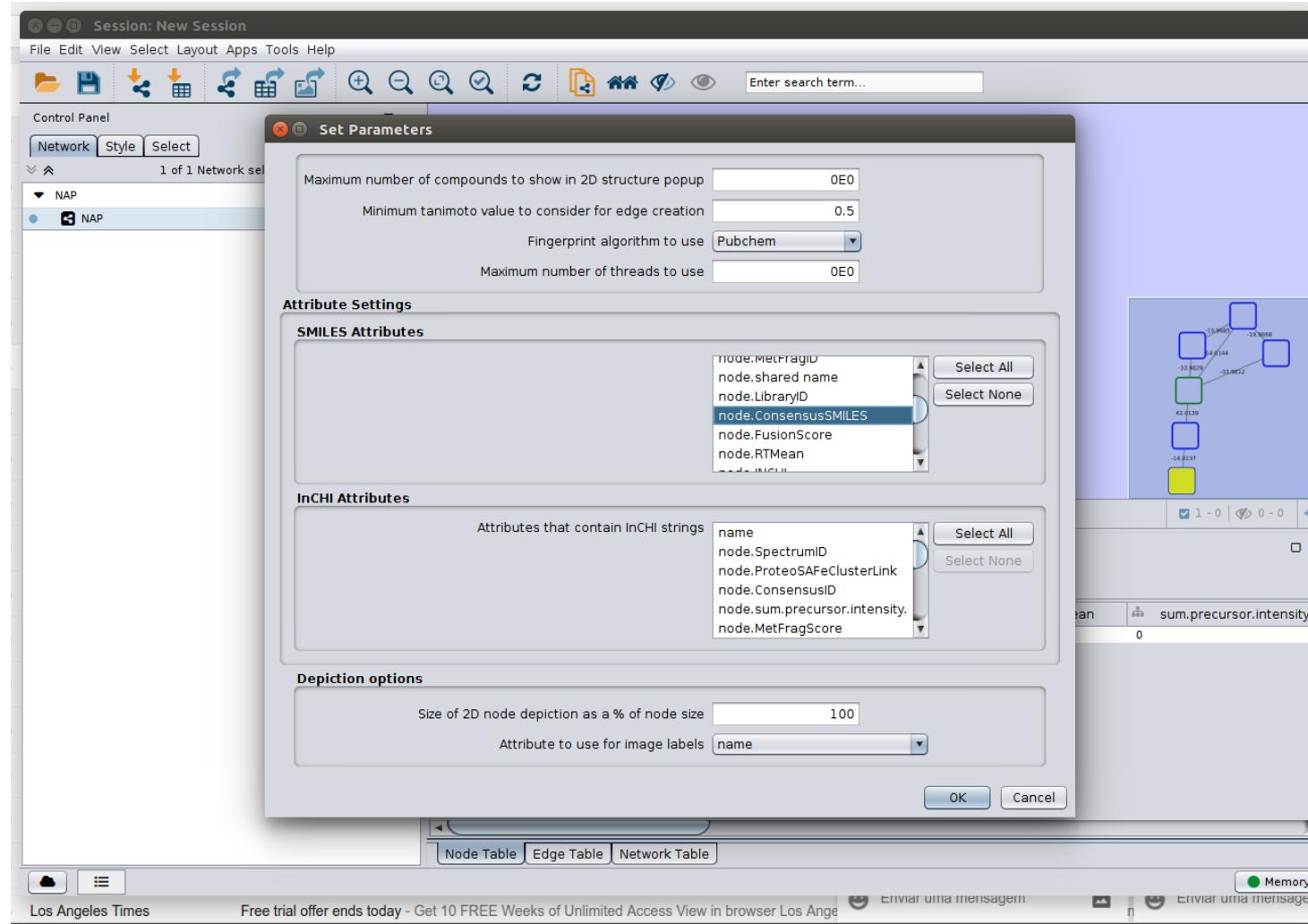
Install the chemViz2 app on menu Apps



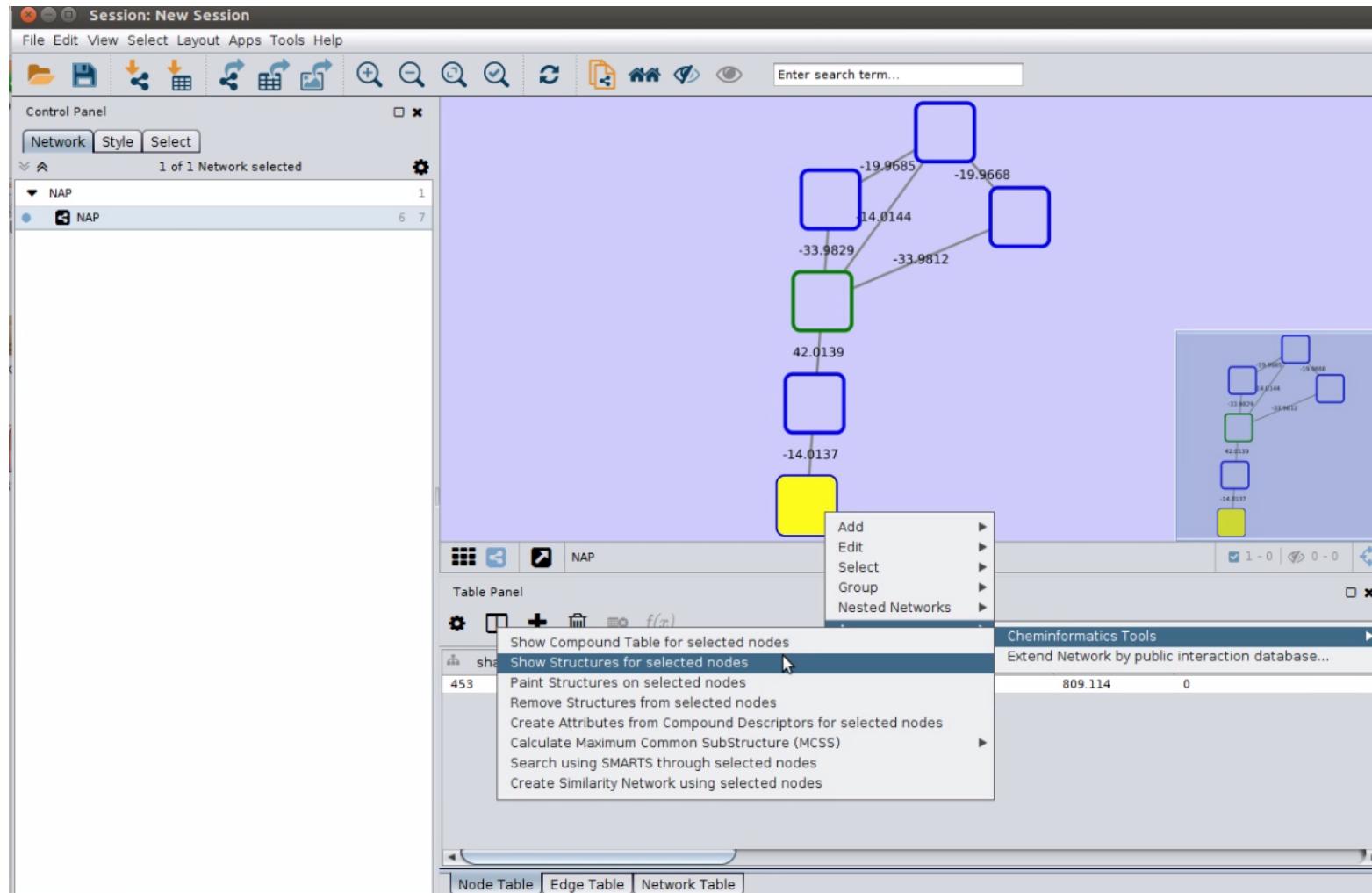
**Candidate structures are available to each ranking strategy.
To choose which structures to dysplay go to:
Apps > Cheminformatics Tools > Settings...**



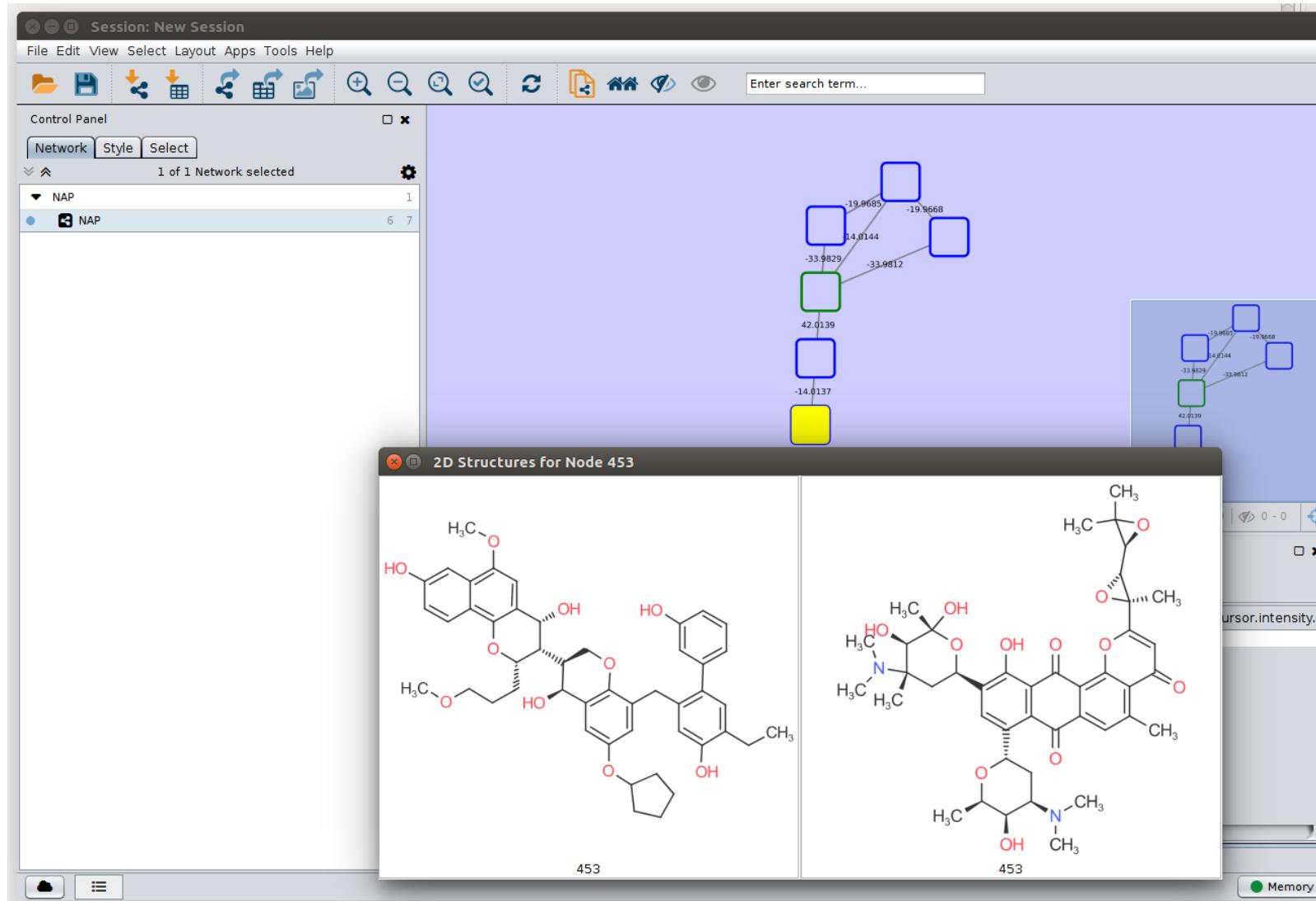
Select the SMILES structure to be displayed, in the example node.ConsensusSMILES



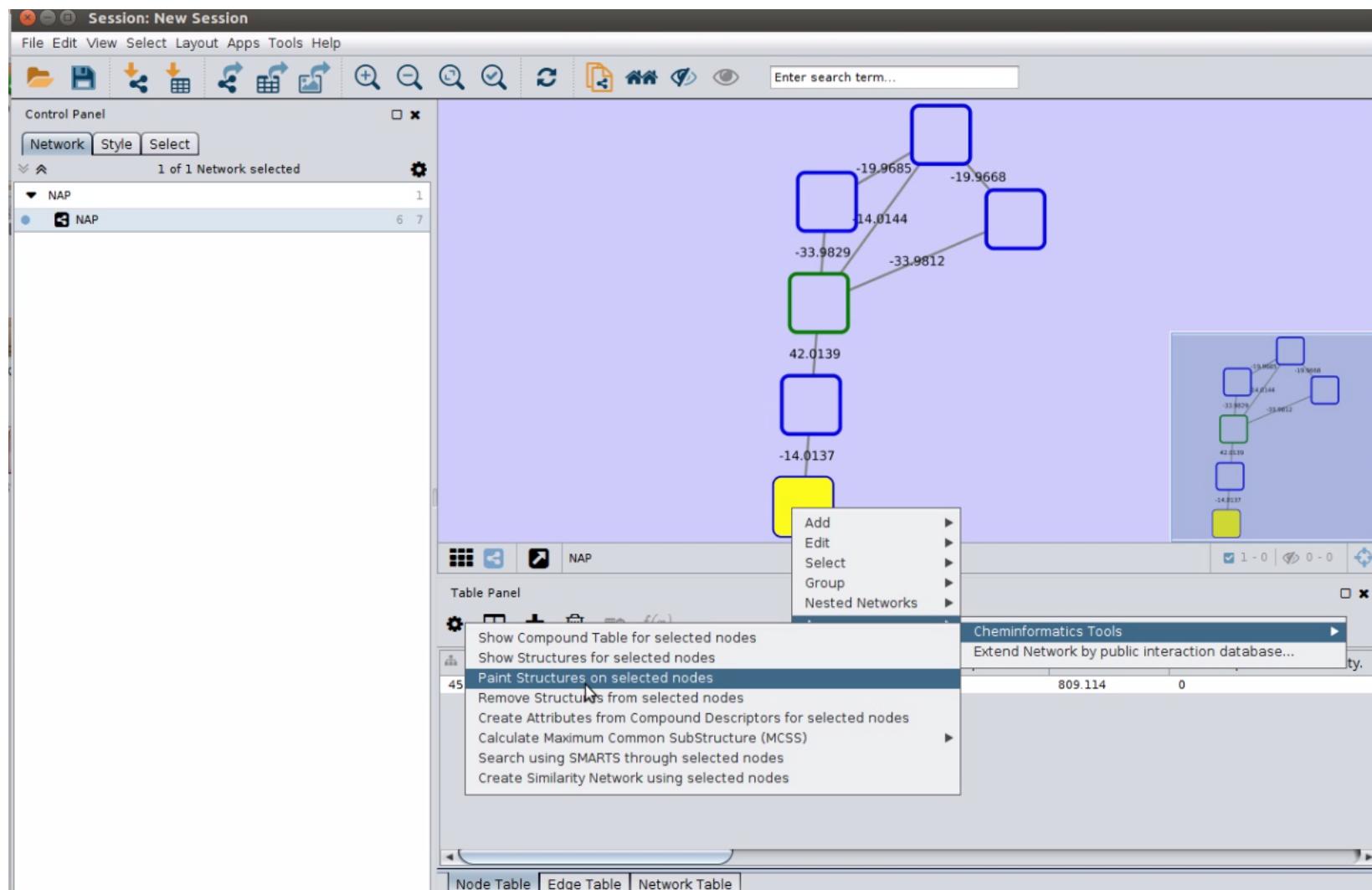
**To display a set of candidate structures for a given cluster node
right click on one node and do:
Apps > Cheminformatics Tools > Show Structures for selected nodes**



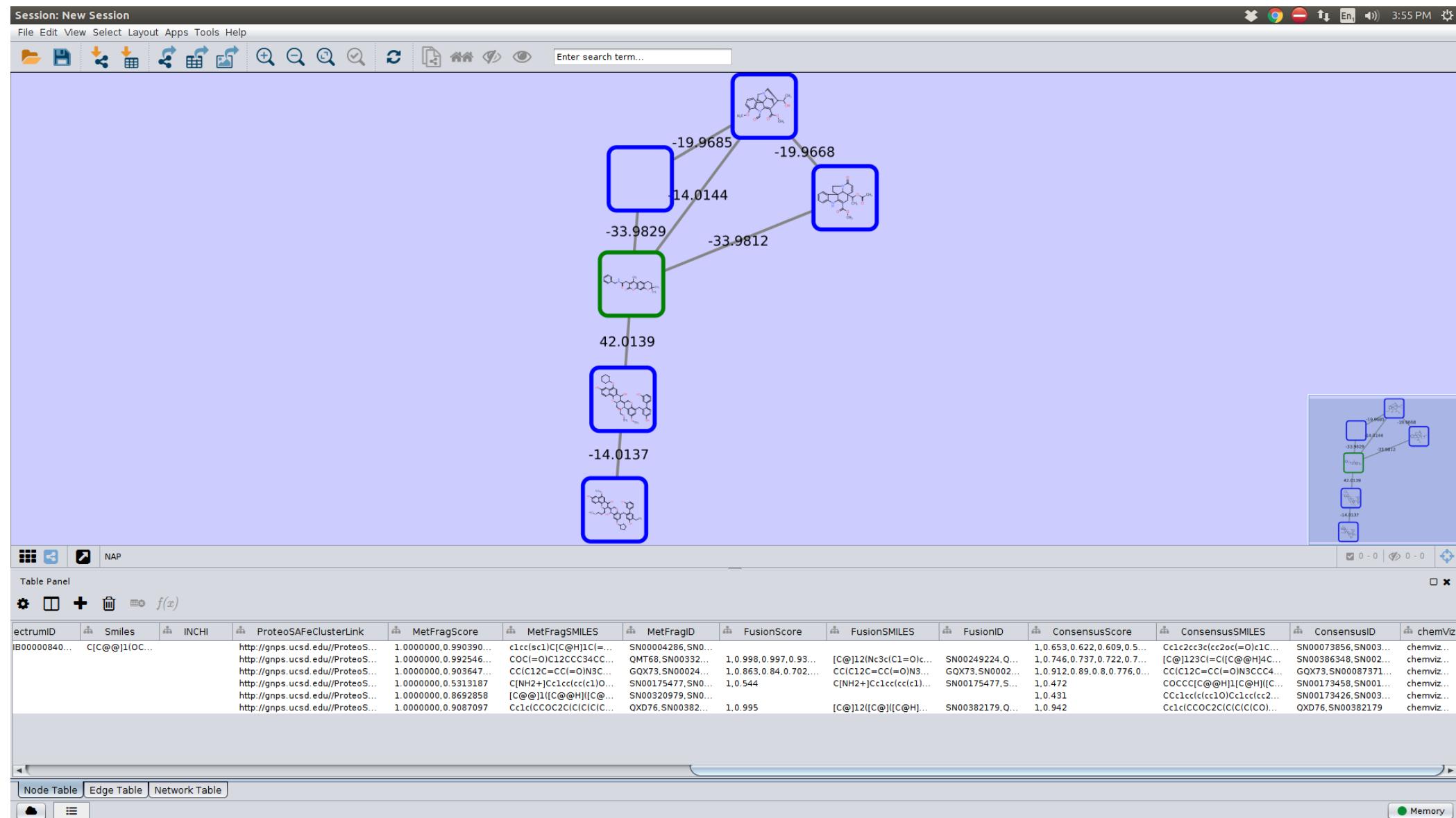
To display a set of candidate structures for a given cluster node
right click on one node and do:
Apps > Cheminformatics Tools > Show Structures for selected nodes



To display structures for a given group of cluster nodes
Select one or more nodes right click on the selection and do:
Apps > Cheminformatics Tools > Paint Structures for selected nodes



It may be necessary multiple selections of the SMILES source to display Spectral Library search structure (green nodes) and MetFrag, Fusion and Consensus (blue, for in silico fragmentation candidate)



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