

User Interface

The screenshot shows the Center for Computational Mass Spectrometry (CCMS) user interface. At the top, there's a navigation bar with links for Logout, Update Profile, Jobs, General Info, UCSD Proteomics, Future Tools, Demo, and Contact. A red "BETA" badge is in the top right corner. Below the navigation is a header with the CCMS logo, the text "Computer Science and Engineering University of California, San Diego", and "Center for Computational Mass Spectrometry". A mass spectrum plot is visible in the background.

Workflow Selection

Workflow: NAP_CCMS2

Title: nap_interface_test

Search Protocol: None

Reset Form | Save as Protocol

File Selection

GNPS job ID: ffa69e06fd8

Number of a cluster node: 1240

N first candidates for consensus score: 10

Accuracy for exact mass candidate search.: 15

Acquisition mode: Positive

Structure databases: HMDB

User provided database: Select Input Files

Maximum number of candidates structures in the graph.: 1

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

Whether to use the *fusion* ranking to select the *n* first candidates of neighbors

Cosine threshold around the selected node

Cosine value to subselect inside a cluster: 0.8

Use fusion result for consensus

Adduct ion type: [M+Na]

Compound class to be selected:

Skip parent mass selection

Whether to skip the candidate structure selection using a mass windows. Only recommended to small databases and or in conjunction of class selection

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

Workflow Submission

Email me at: ridasilva@ucsd.edu

Submit

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Workflow Selection

- Workflow: NAP_CCMS2
- Search Protocol: None
- Reset Form
- Save as Protocol

Title: nap_interface_test

File Selection

- GNPS job ID: ffa69e06fd8
- Number of a cluster node: 1240
- Cosine value to subselect inside a cluster: 0.8
- Use fusion result for consensus
- N first candidates for consensus score: 10
- Accuracy for exact mass candidate search.: 15
- Acquisition mode: Positive
- Structure databases: HMDB
- User provided database: Select Input Files
- Maximum number of candidates structures in the graph.: 1

Workflow Submission

Email me at ridasilva@ucsd.edu

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

CCMS ProteoSAFE File/Resource Manager - Google Chrome

proteomics2.ucsd.edu/ProteoSAFE/upload.jsp

Select Input Files Upload Files Share Files

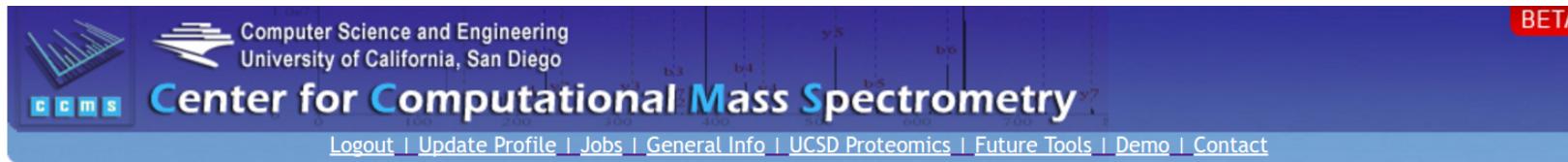
Select Upload Folder

File Drag and Drop

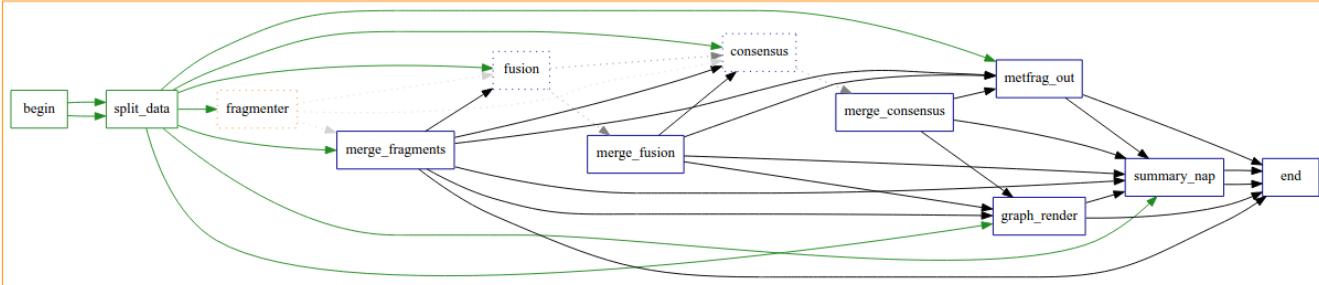
Drop Files Here To Upload

- [Task 50ec...] - "AMGagain"
- [Task fb05...] - "nap_ccms_t29"
- CCMS_ProteomeDatabases
- CCMS_School_2017
- CCMS_SpectralLibraries
- [Dataset MSV000078556] - "GNPS - Topobiographical molecular analysis"
- [Dataset MSV000078568] - "GNPS_Dorrestein_Gerwick_Cyanobacteria"
- [Dataset MSV000078622] - "GNPS - 3D molecular analysis of skin surfaces"
- [Dataset MSV000078727] - "GNPS_Bidens32bits_conversion"
- [Dataset MSV000078745] - "gnps_UntargetedMetabolicProfilingAsp"
- [Dataset MSV000078768] - "GNPS_L_E_UEC-127_MS2"
- [Dataset MSV000078770] - "GNPS_VERN_TOMEM-1408_MS2"
- [Dataset MSV000078860] - "GNPS Bacteria CB0028 associated to Adipose"
- [Dataset MSV000078879] - "GNPS_Test_submission"
- [Dataset MSV000078881] - "GNPS_Teobroma cacao"
- [Dataset MSV000078889] - "GNPS_plant_extracts"
- [Dataset MSV000078899] - "GNPS_Lychnophora"
- [Dataset MSV000079054] - "GNPS INSPIRE Soil Microbes exposed to Root Exudates on +/- Pi media B3R1T1"
- [Dataset MSV000079001] - "GNPS_SS_nootriter"

Workflow monitor



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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

Computer Science and Engineering
University of California, San Diego
Center for Computational Mass Spectrometry

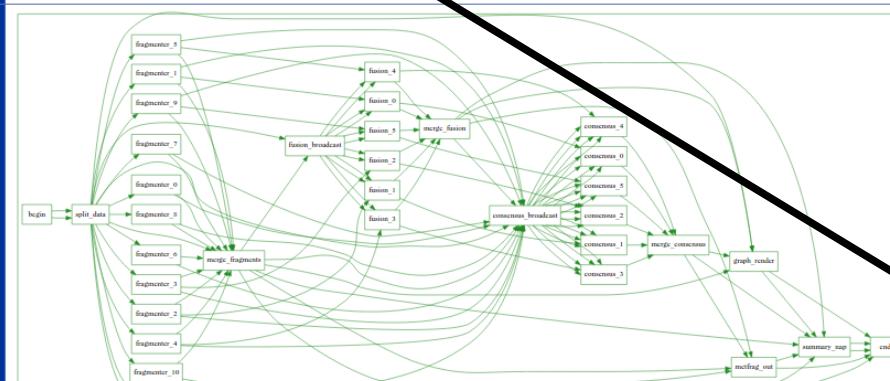
Logout | Update Profile | Jobs | General Info | UCSD Proteomics | Future Tools | Demo | Contact

[Back to main page](#)

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]

Computer Science and Engineering
University of California, San Diego
Center for Computational Mass Spectrometry

Logout | Update Profile | Jobs | General Info | UCSD Proteomics | Future Tools | Demo | Contact

[Back to main page](#) [Back to status page](#) [Collapse all](#)

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

nap_interface_test

Hits 1 - 6 out of 6

Go to Go

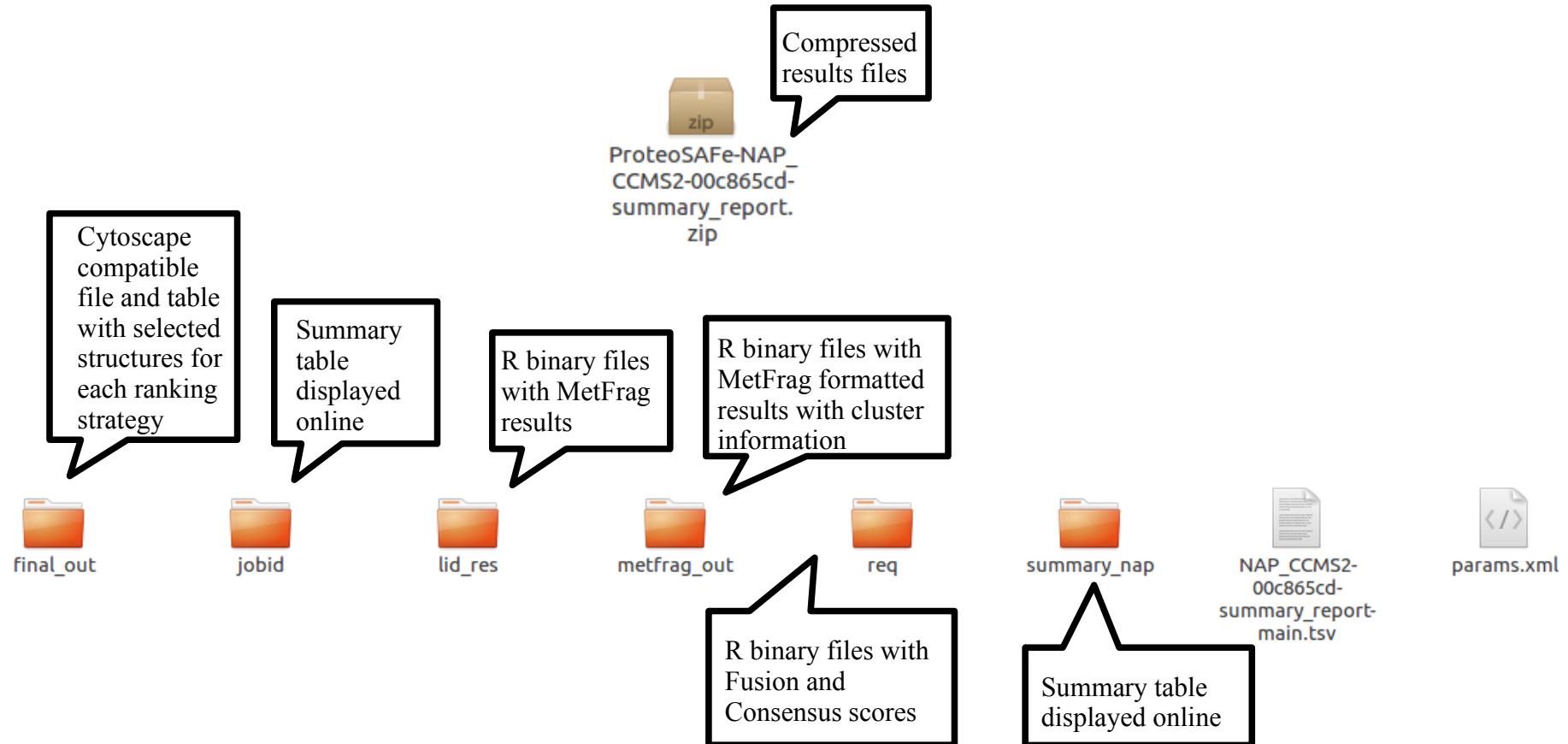
Select columns

cluster.index	Parent Mass	RT	LibraryID	MetFragID	MetFragSC
1	34	827.339	907.145	euphorboidinT	SN00004286#SN00023815#SN00025151#SN00132116#CCMSLIB00000578251#SN00061408
2	40	841.353	1069.950	N/A	QMT68#SN00245602#CFG34#SN00247561#PKG63#SN00353054#LGT03#SN00064161#SN00275612#SN00298127#SN00253343#CDP26
3	46	861.320	975.383	N/A	GQX73#SN00024393#SN00139900#SN00070780#SN00074249#QXM36#SN00098223
4	426	785.325	645.822	N/A	
5	453	799.339	809.114	N/A	
6	549	861.322	978.120	N/A	

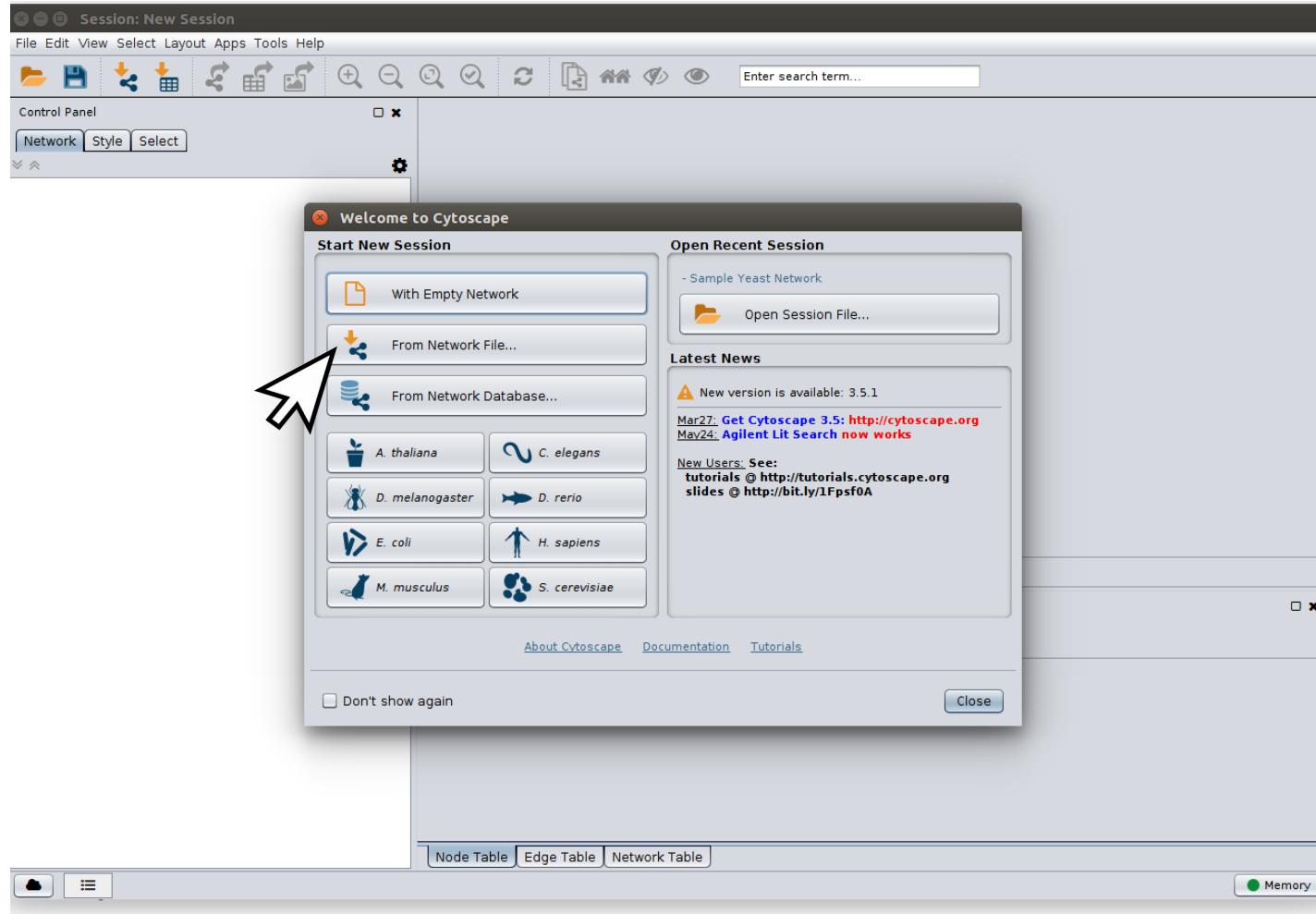
Summary table with the results of IDs and Super Class of compounds inside the group of the first ranking structure by each scoring strategy

Download Results

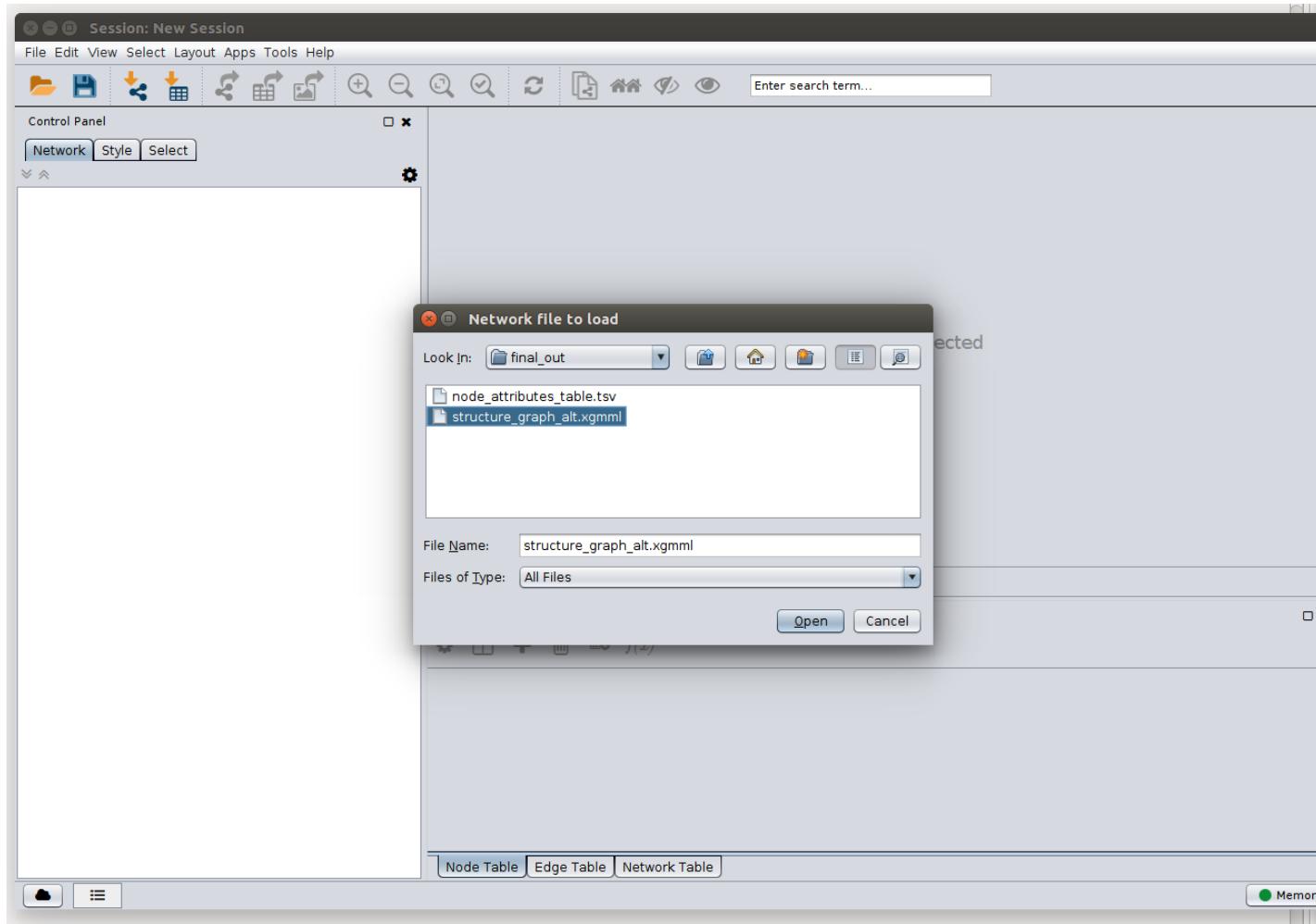
Result Files



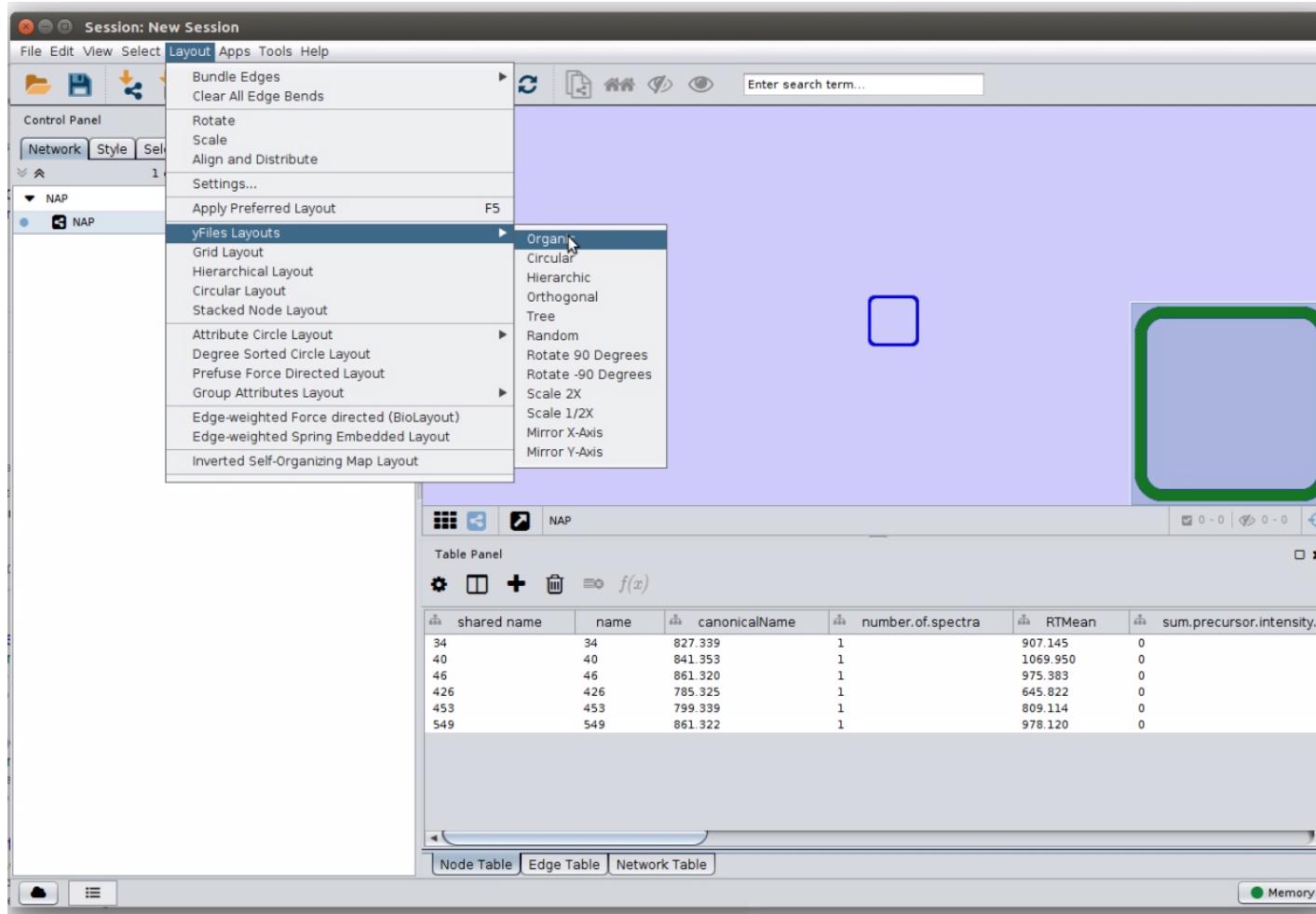
Use Cytoscape From Network File import function



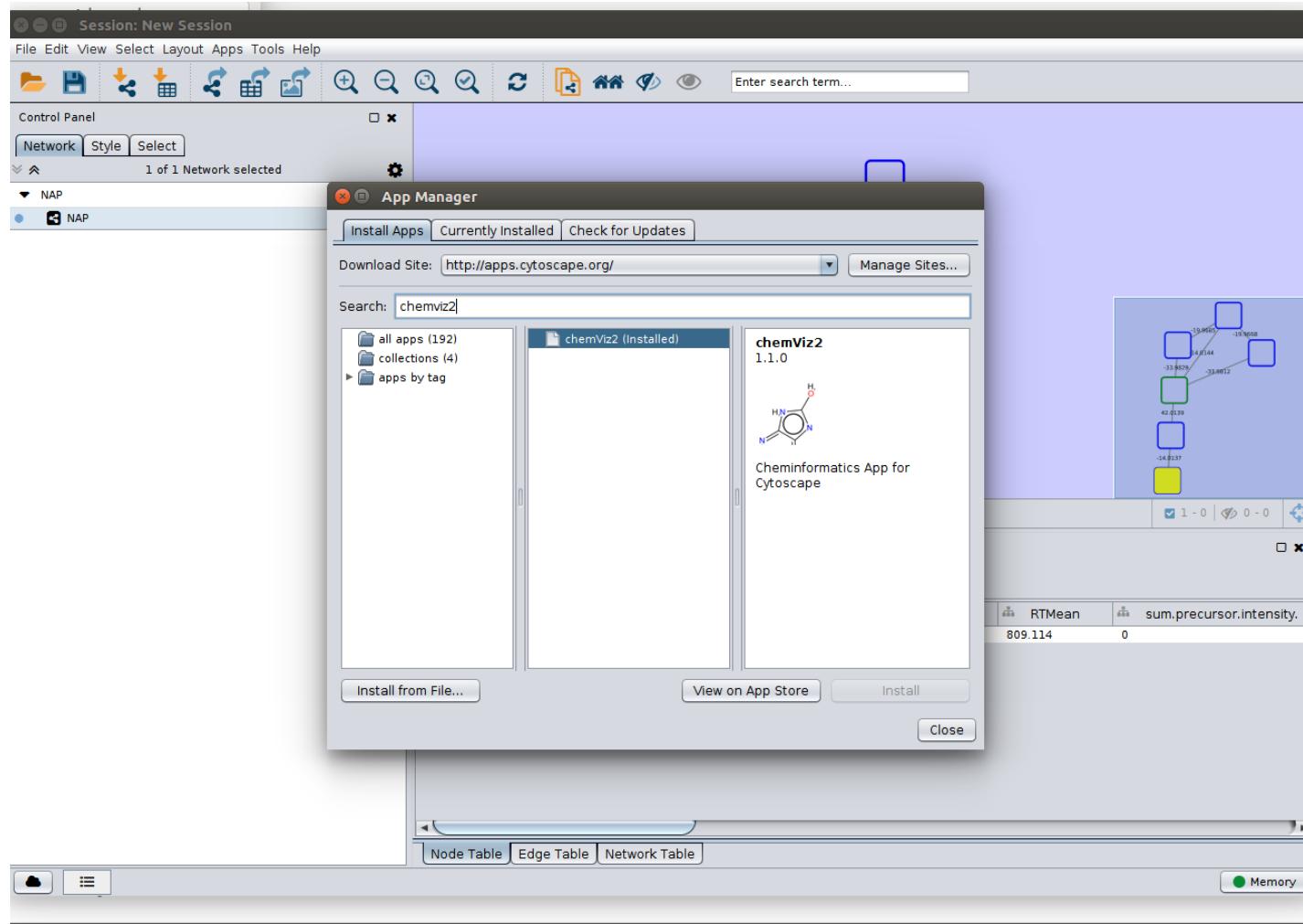
Import the file *structure_graph_alt.xgmm* inside *final_out* folder



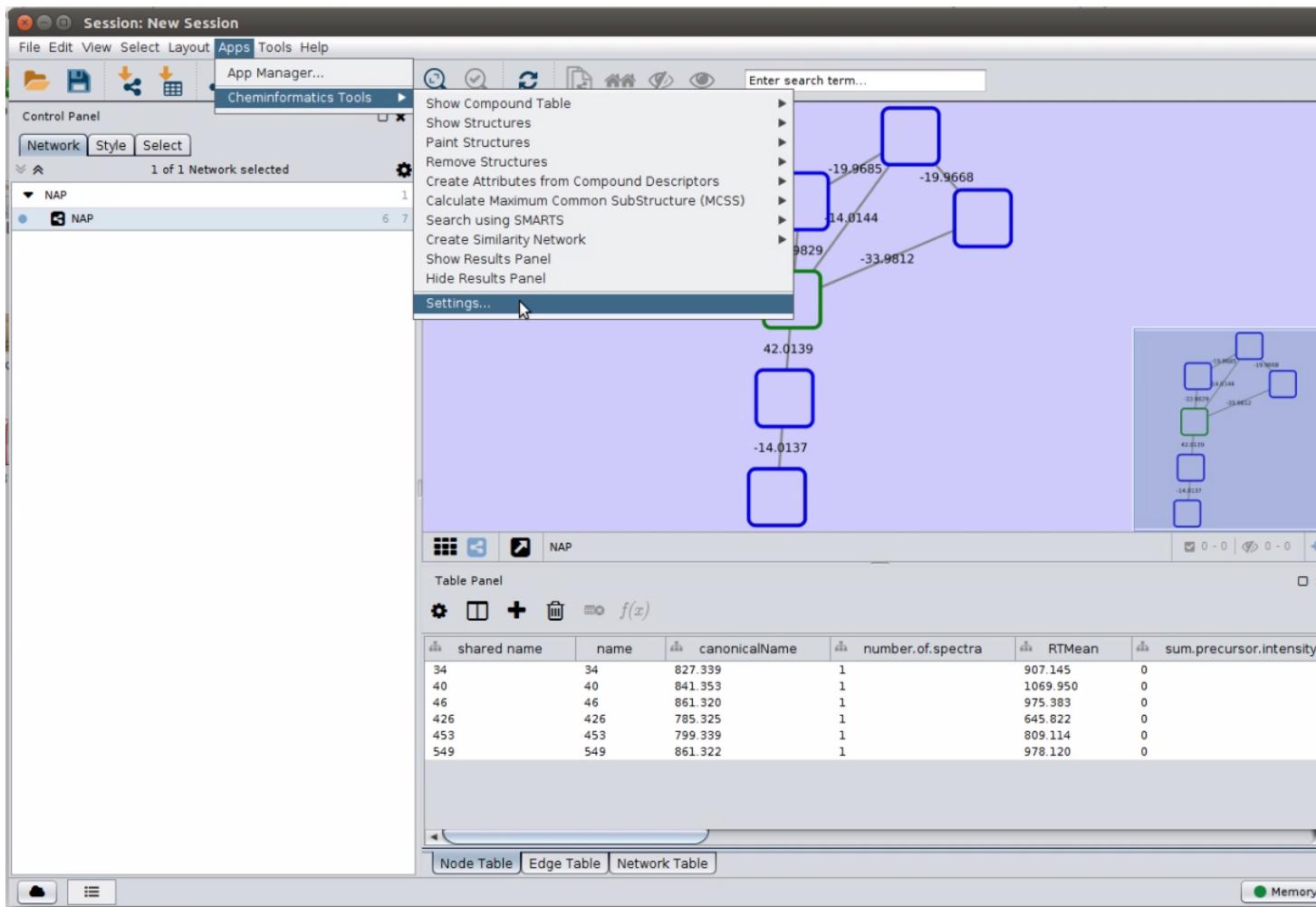
Apply a layout to spread the nodes and help visualization



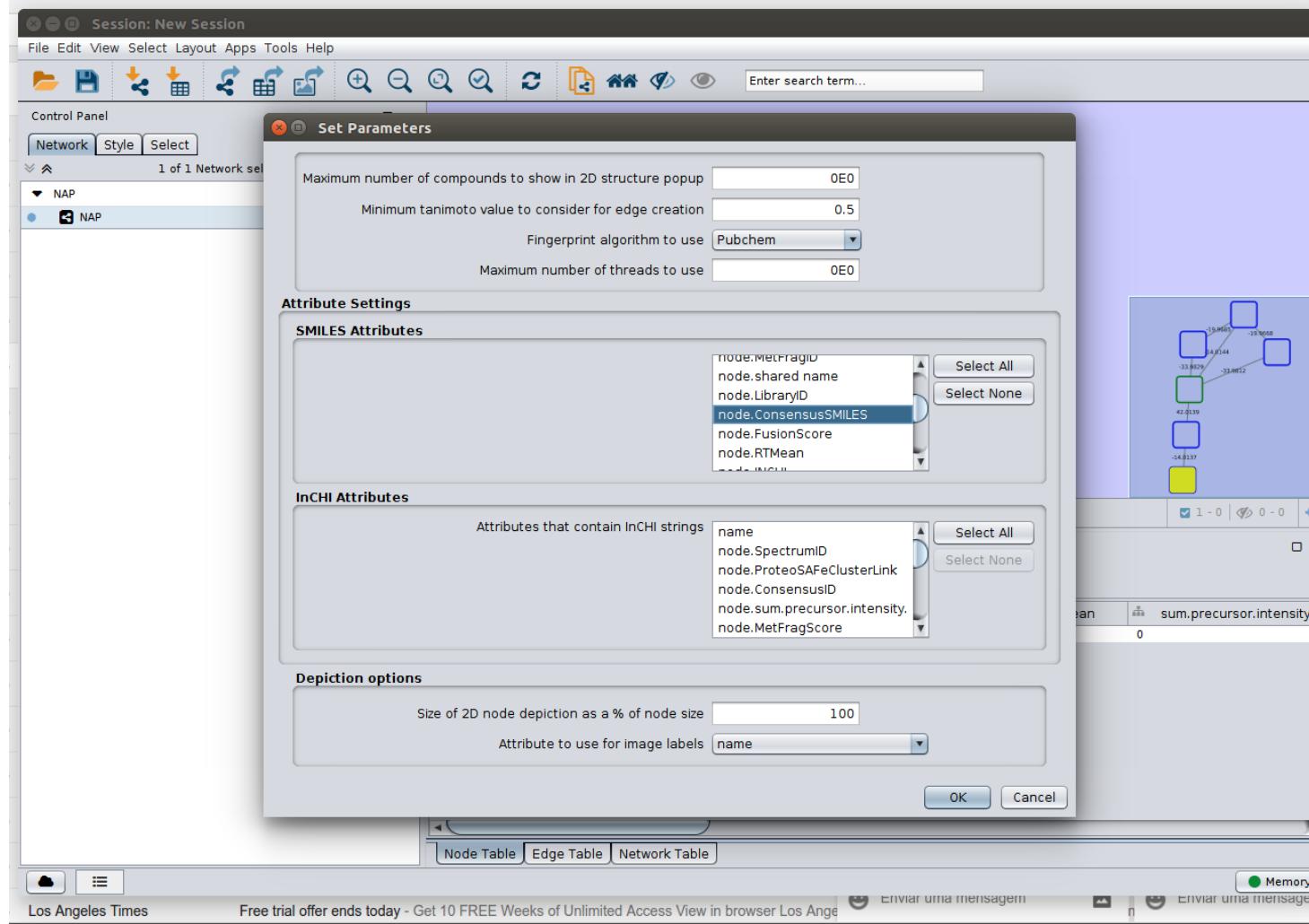
Install the chemViz2 app on menu Apps



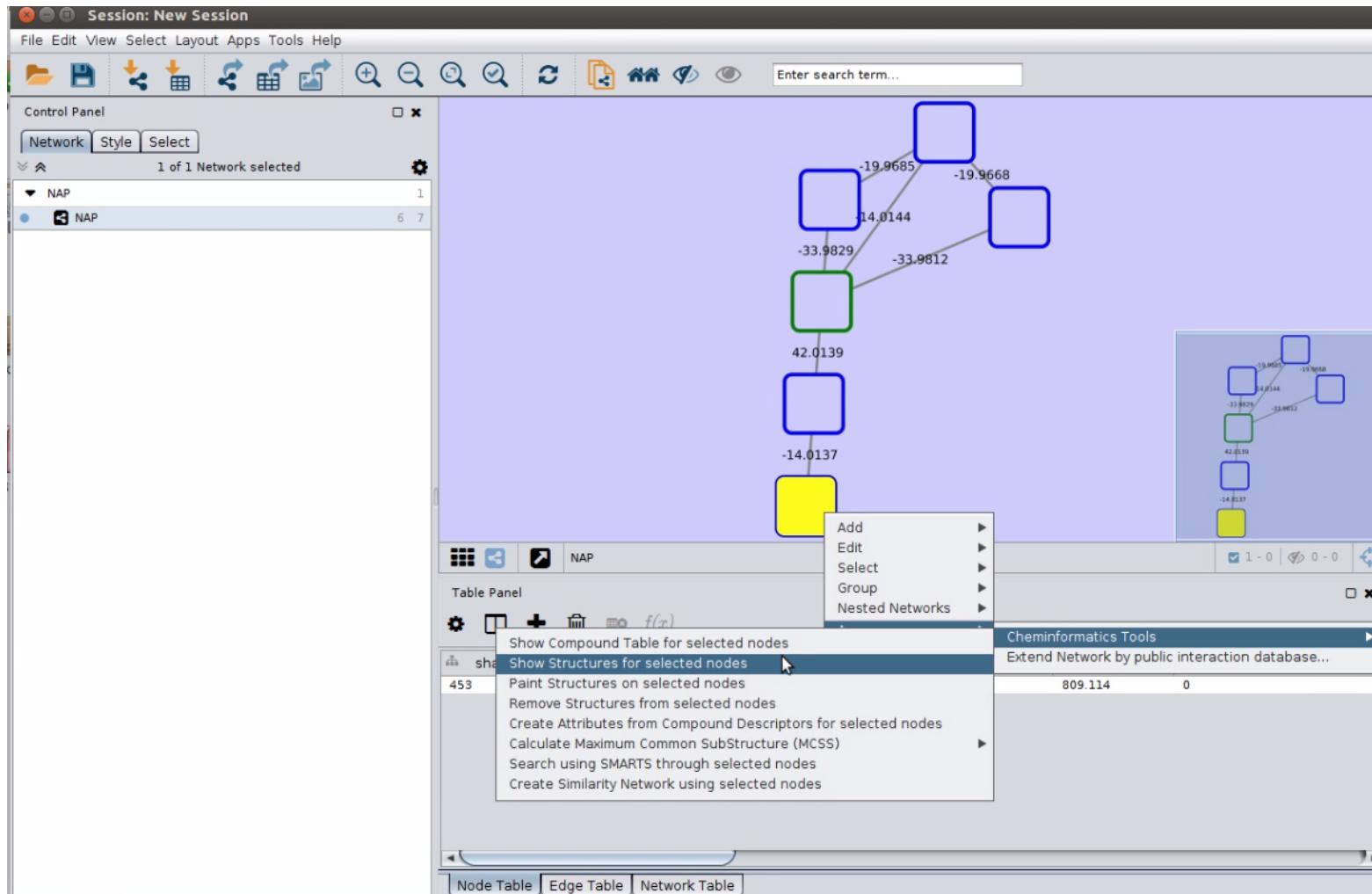
**Candidate structures are available to each ranking strategy.
To choose which structures to dysplay go to:
Apps > Cheminformatics Tools > Settings...**



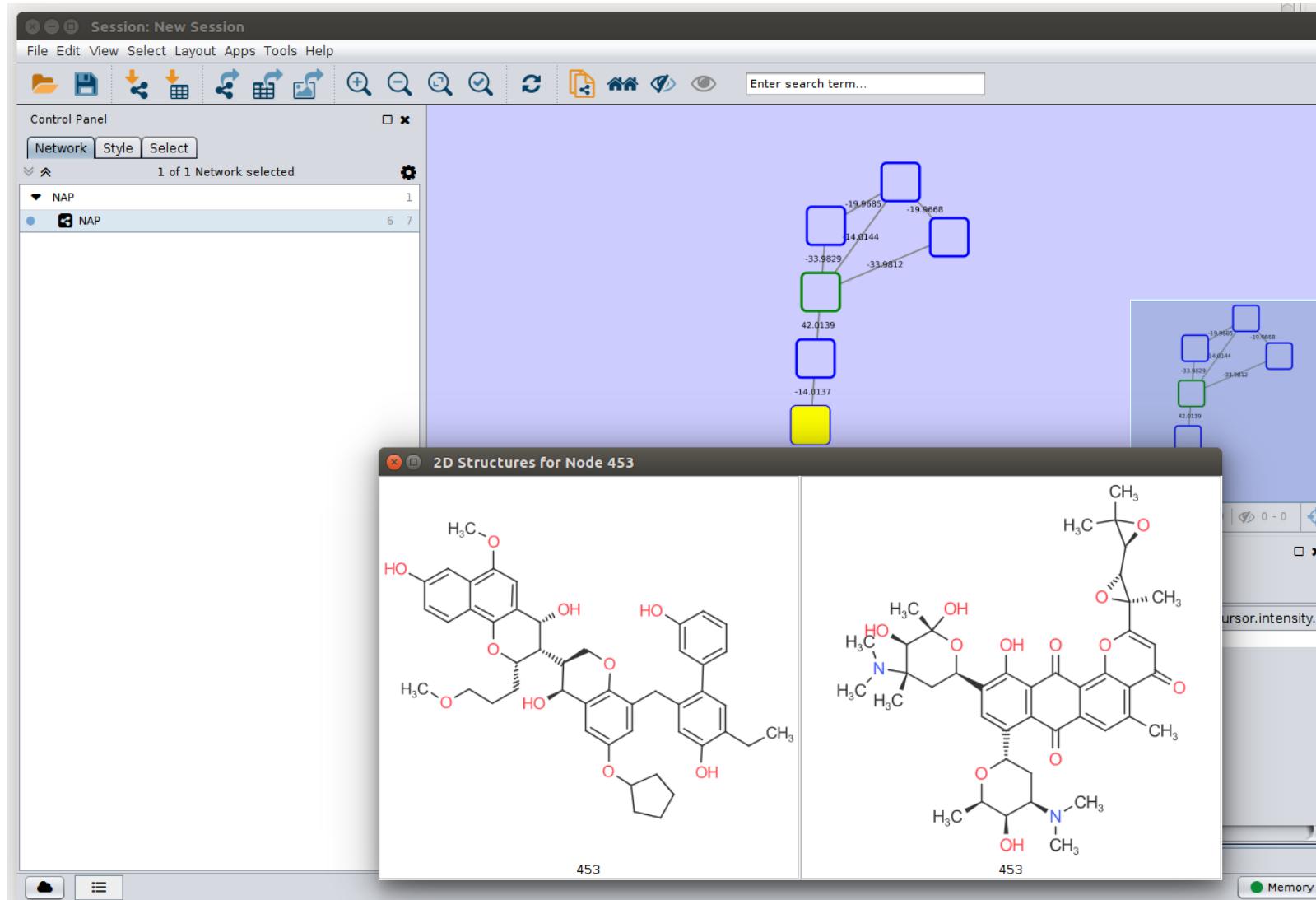
Select the SMILES structure to be displayed, in the example node.ConsensusSMILES



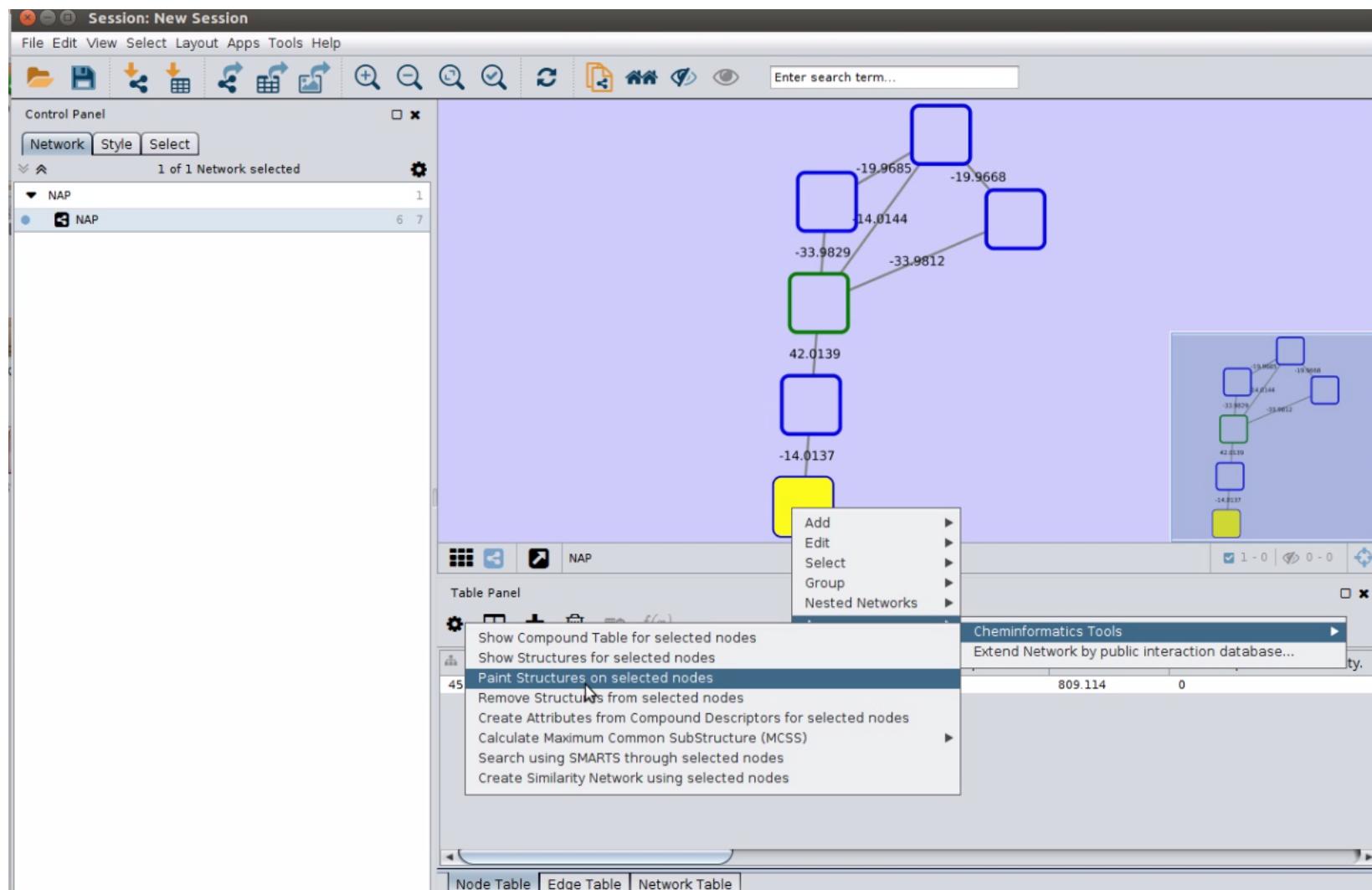
**To display a set of candidate structures for a given cluster node
right click on one node and do:
Apps > Cheminformatics Tools > Show Structures for selected nodes**



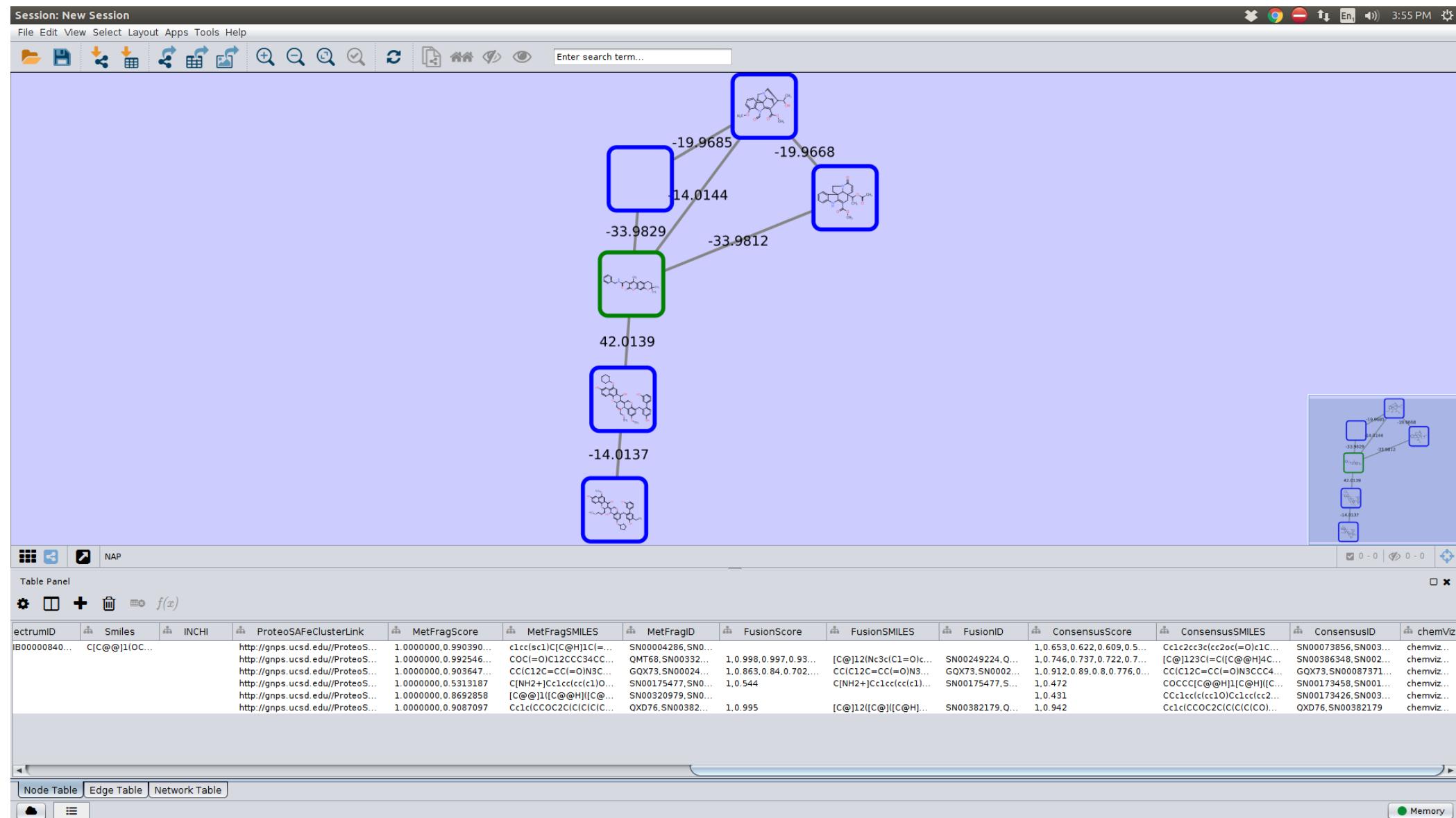
**To display a set of candidate structures for a given cluster node
right click on one node and do:
Apps > Cheminformatics Tools > Show Structures for selected nodes**



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)



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)

