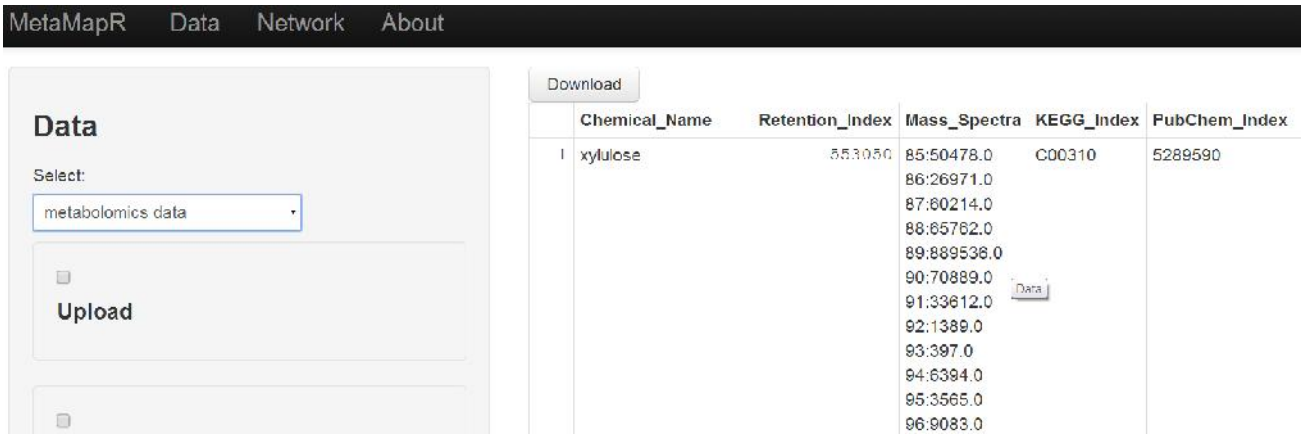
To make networks using MetaMapR v1.2.1 (https://github.com/dgrapov/MetaMapR)

You can take a look at **the data format required** by downloading the "metabolomics data".

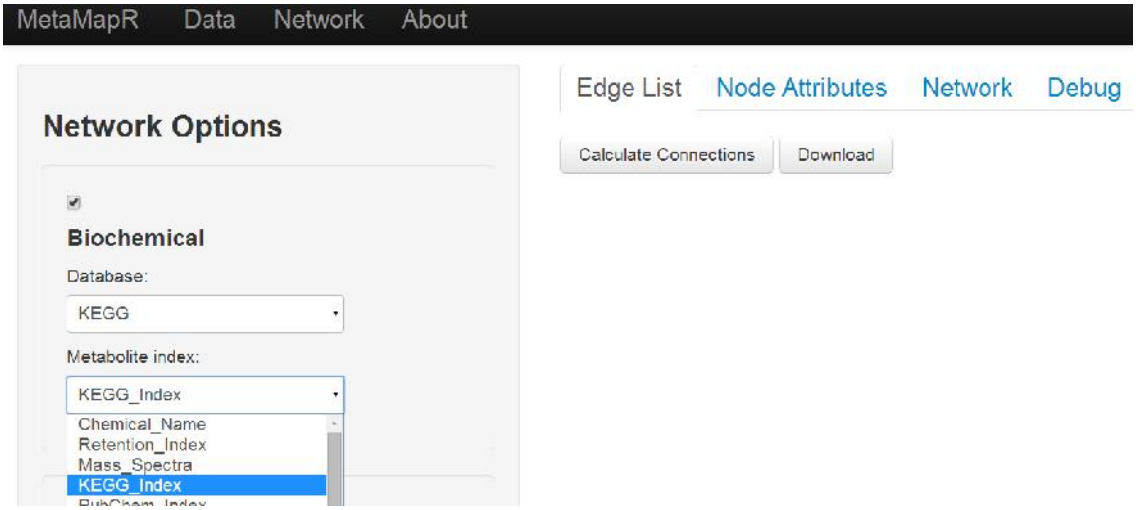


The data simply need to be in a csv. (column names help).

Chemical_Name	Retention_Index	Mass_Spectra	KEGG_Index	PubChem_Index	Main	Sample.1	Sample.2	Sample.3	Sample.4	Sample.5
xylulose	553050	85:50478.0 86:26971	C00310	5289590	0	614	858	785	1736	608
xylitol	566570	86:588.0 87:117.0 88	C00379	6912	0	5375	7345	5186	7934	4080
xanthosine	924754	86:74.0 88:56.0 93:1.	C01762	64959	0	63	19	22	20	34
xanthine	702301	85:1361.0 86:1949.0	C00385	1188	0	885	2816	464	2529	2138
valine	809905	85:2890.0 86:6277.0	C00183	6287	0	97956	522008	128448	102052	101682
uridine	856953	85:2472.0 86:1478.0	C00299	6029	0	383	1444	431	273	813
uridine	813744	99:55.0 100:209.0 10	C02067	15047	0	17344	15406	9883	51908	8475
uric acid + myo-inositol	730534	85:1183.0 86:635.0 8	C00366	1175	0	6215	20217	7131	9672	16398
urea	325479	85:646.0 86:721.0 87	C00086	1176	0	335020	158277	425732	662227	403793
uracil	385903	85:620.0 86:348.0 87	C00106	1174	0	2052	3956	1862	3407	3095
tyrosine	670802	86:117.0 91:15.0 92:	C00082	6057	1	121190	95798	127310	65341	152554
tryptophan	781209	85:32.0 86:353.0 88:	C00078	6305	0	154453	80404	136283	70363	118829
triethanolamine	530879	87:141.0 88:120.0 90	C06771	7618	0	74	4957	361	7987	126
trehalose	947837	86:85.0 89:2588.0 90	C01083	7427	0	748	3745	212	780	591

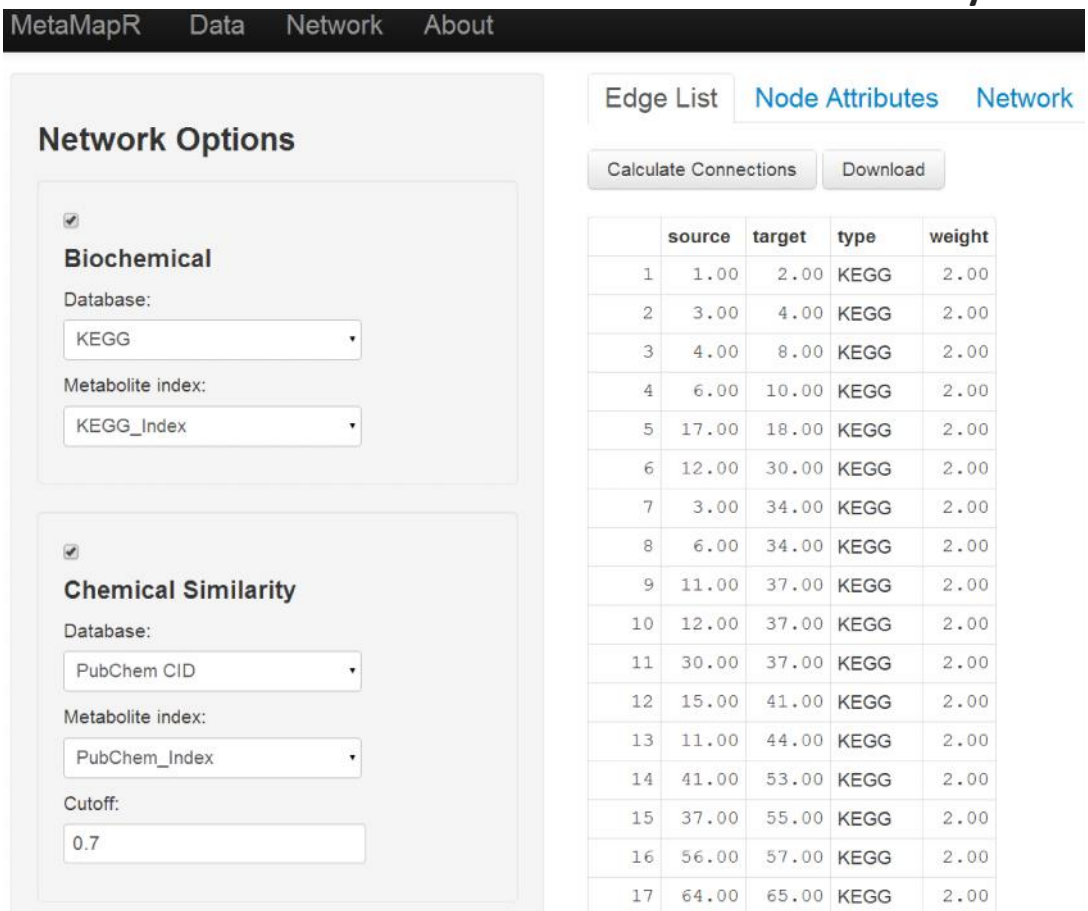
To make the networks you need to select which column in the data corresponds to the needed object.

For **biochemical interactions** you need KEGG IDs. Here is an example of this selection (I merely select the column in the data with KEGG IDs). If you don't have theses then you can translate from name to KEGG or other on the data--> translate tab.



Once you made the selection hit the calculate connections button to get the edge list. Download this object to generate the network in Cytoscape. You will see how the node attributes match the edge IDs in the node attributes tab.

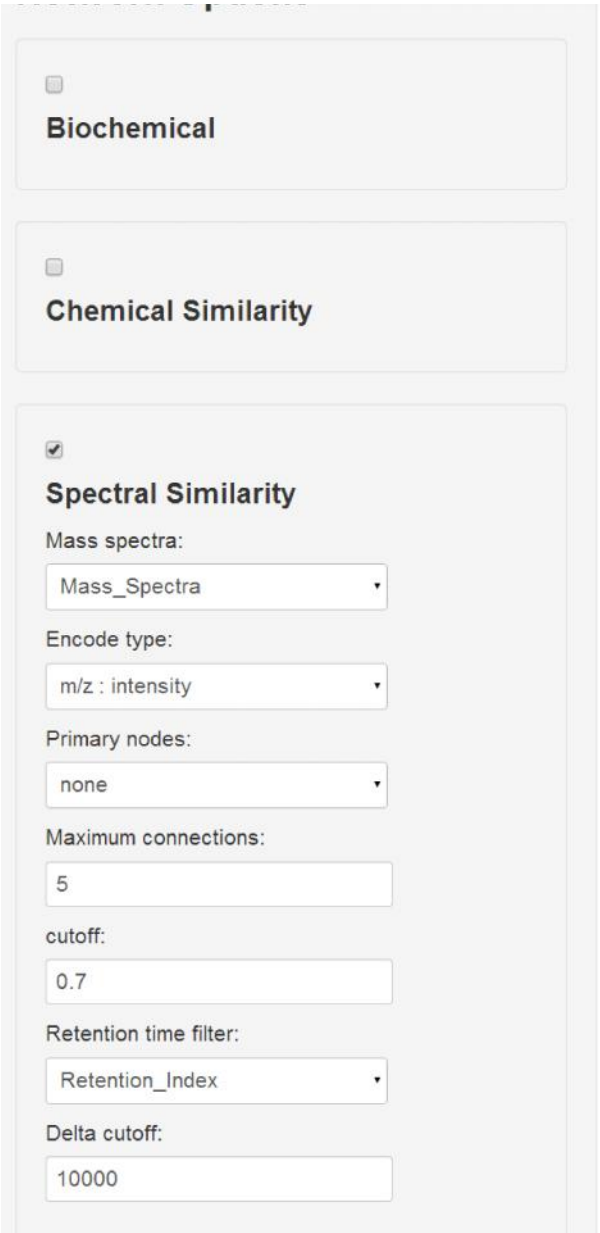
Here are the choices to **make biochemical and structural similarity** networks.



	source	target	type	weight
1	1.00	2.00	KEGG	2.00
2	3.00	4.00	KEGG	2.00
3	4.00	8.00	KEGG	2.00
4	6.00	10.00	KEGG	2.00
5	17.00	18.00	KEGG	2.00
6	12.00	30.00	KEGG	2.00
7	3.00	34.00	KEGG	2.00
8	6.00	34.00	KEGG	2.00
9	11.00	37.00	KEGG	2.00
10	12.00	37.00	KEGG	2.00
11	30.00	37.00	KEGG	2.00
12	15.00	41.00	KEGG	2.00
13	11.00	44.00	KEGG	2.00
14	41.00	53.00	KEGG	2.00
15	37.00	55.00	KEGG	2.00
16	56.00	57.00	KEGG	2.00
17	64.00	65.00	KEGG	2.00

Alternatively you could make mass spectral similarity networks (or mix and match any connections).

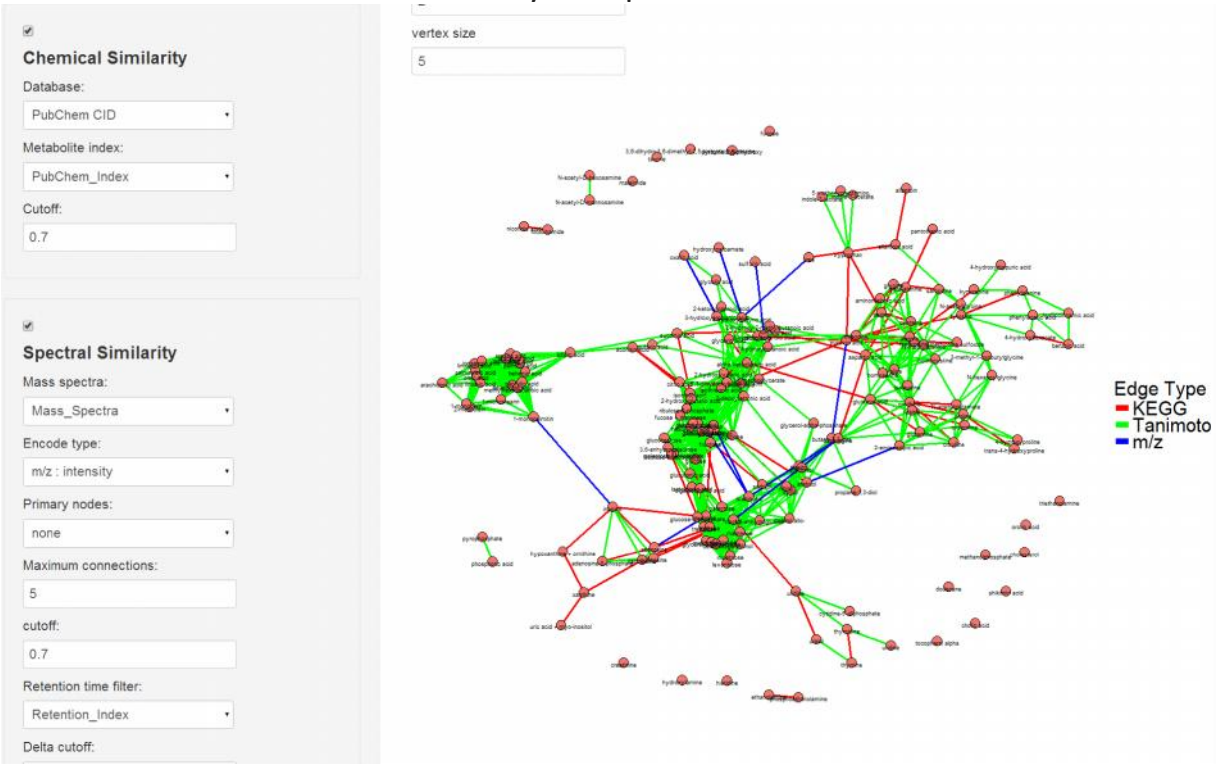
To make **mass spectral similarity** networks you need data encoded like we do for BinBase and optionally supply the retention times. The Delta cutoff makes sure compounds are both spectrally similar and have similar retention times (in the window 10,000 units fro each other in the example above). You can also optionally give an index of 1s and 0s for (1,0,1,...) for which metabolites have names. This way only connections from unknown to known will be returned.



Calculate Connections | Download

	source	target	type	weight
10	14.00	131.00	m/z	0.78
27	9.00	156.00	m/z	0.78
39	6.00	124.00	m/z	0.84
42	23.00	161.00	m/z	0.96
56	24.00	151.00	m/z	0.74
104	37.00	134.00	m/z	0.84
155	67.00	123.00	m/z	0.74
161	51.00	160.00	m/z	0.93
165	35.00	142.00	m/z	0.84
175	73.00	74.00	m/z	0.88
186	71.00	143.00	m/z	0.98
231	54.00	74.00	m/z	0.76
245	85.00	175.00	m/z	0.74
252	91.00	156.00	m/z	0.83
259	77.00	131.00	m/z	0.91
323	88.00	141.00	m/z	0.88
402	139.00	143.00	m/z	0.73
405	34.00	139.00	m/z	0.88
408	142.00	172.00	m/z	0.77
415	143.00	164.00	m/z	0.72
438	160.00	161.00	m/z	0.93
453	171.00	173.00	m/z	0.96
457	174.00	176.00	m/z	0.82

To **build a network** make sure you calculate the edge list first or make the need selections from the data, then use network tab to plot (may need to open options and hit plot to update). The network itself is more for overview and tuning the inputs, I would make the real networks in Cytoscape.



Recommendations and ~FAQ:

I would run MetaMapR locally and not use the server which has upload size limitations and only allows 1 user at a time.

Run locally by down loading the zip and use runApp("filepath") command or the shiny::runGitHub('MetaMapR','dgrapov') which downloads fresh copy eachtime.

The "error: attempt to set an attribute on NULL" happens when the program initializes, but should go away in a couple of seconds (could take longer on slower computers).

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