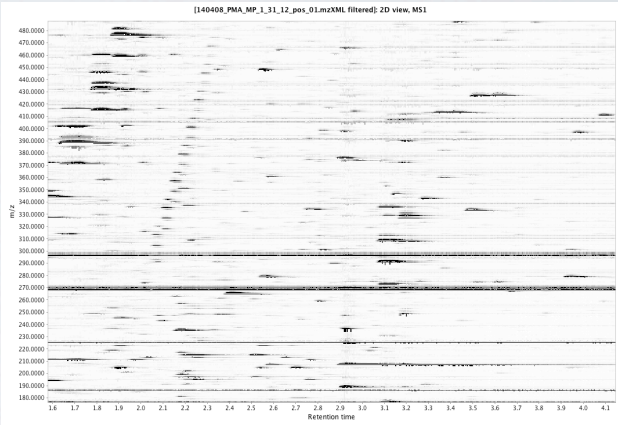
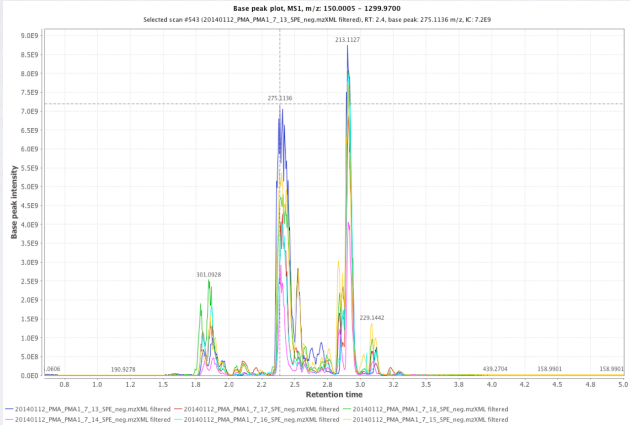
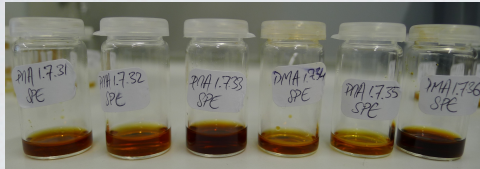
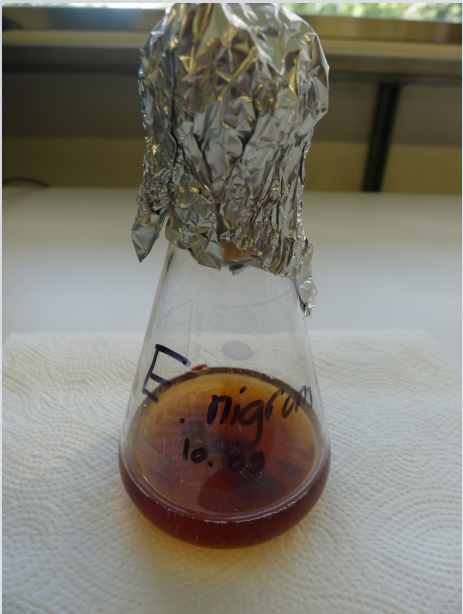




Dereplication and databases (part2) : ***molecular networking tools***

LC-MS et substances naturelles
07-05-2015

Pierre-Marie Allard
Université de Genève



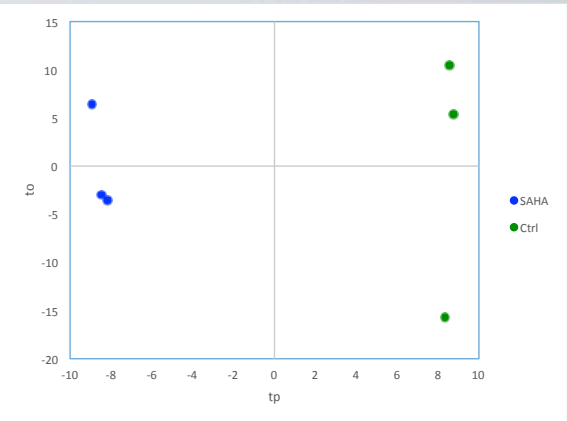
ID	Average		Identity	Co...	Peak shape	140408_PMA...		140408_PMA...		140408_PMA...		140408_PMA...		140408_PMA...		14040...
	m/z	Ret...				Hel...	Area	Hel...	Area	Hel...	Area	Hel...	Area	Hel...	Area	
106	353.2476	3.1				6.4E7	4.4E7	3.8E7	1.8E7	3.9E7	1.8E7	3.5E6	3.7E6	8.3E6	1.2E7	4
63	286.1415	2.9	SAHA_IM+Na-HI 21.9825...			6.1E7	6.7E7	3.8E7	1.9E7	6.1E7	9.1E7			2.0E6	2.1E6	1
94	162.0550	1.9	MEDIA_6-Hydroxy-JH-ind...			5.1E7	1.2E8	3.3E7	2.5E7	2.0E7	6.9E7	1.1E8	3.6E8	9.2E7	2.8E8	4
134	402.1743	2.5				3.2E7	2.5E7	2.1E7	2.7E7	3.2E7	1.7E7					
102	277.2163	3.7	9,14-Octadecadien-12-yn...			4.7E7	5.1E7	3.3E7	2.7E7	5.3E7	4.8E7	2.6E7	2.3E7	4.2E6	3.8E6	5
113	205.0860	2.7	4-Hydroxy-5,6-dodecadi...			4.3E7	4.9E7	4.2E7	3.0E7	3.7E7	1.8E7	9.4E7	1.5E8	6.2E7	1.1E8	6
120	165.1275	3.7				4.0E7	3.0E7	3.1E7	3.1E7	5.6E7	7.2E7	2.2E7	2.4E7	3.2E6	3.6E6	3
126	433.2840	1.9				3.7E7	0.0E0	6.0E7	3.8E7	3.6E7	0.0E0	1.2E8	5.4E7	3.1E7	0.0E0	7
125	474.2912	2.0				3.9E7	1.9E7	4.2E7	3.8E7	4.3E7	6.3E7	8.0E7	1.2E8	6.0E7	9.3E7	6
129	301.1435	2.8	3-(1,3,5-Heptatrienyl)-3,4...			3.5E7	8.5E6	3.0E7	4.0E7	3.4E7	4.6E7	2.5E7	2.7E7	3.3E7	4.8E7	2
64	837.3552	2.5				8.5E7	1.1E8	3.0E7	4.1E7	7.2E7	7.6E7					
96	357.1891	3.2				4.9E7	7.0E7	3.3E7	4.3E7	4.9E7	4.1E7	2.2E5	5.5E4			3
97	398.3418	2.8	SAHA...			4.9E7	5.0E7	2.8E7	5.0E7	3.3E7	5.1E7	7.8E7	1.1E8	6.3E7	1.1E8	4
99	301.1410	3.9	MEDIA_IM+Na-HI 21.9825...			4.8E7	1.1E8	2.9E7	5.6E7	2.5E7	5.1E7	8.9E7	1.8E8	5.6E7	1.3E8	4
104	460.2747	2.0	MEDIA...			4.6E7	4.2E7	5.1E7	5.6E7	4.0E7	5.2E7	7.3E7	8.1E7	5.4E7	3.7E7	6
118	416.2483	1.9	MEDIA...			4.1E7	3.8E7	4.4E7	6.2E7	3.7E7	5.0E7	5.2E7	7.6E7	4.6E7	6.6E7	4
91	266.1581	2.2				5.3E7	7.7E7	5.3E7	6.4E7	1.7E8	4.0E8	1.8E5	4.2E4	2.5E5	3.2E5	2
123	307.1654	2.5	Metacytolin			3.9E7	5.6E7	6.8E7	6.8E7	4.1E7	4.0E7	4.2E5	3.0E5	3.3E5	1.9E5	3
142	249.1598	2.3	SAHA...			3.1E7	0.0E0	5.4E7	6.8E7	3.9E7	4.8E7	9.9E5	1.2E6	7.8E5	1.0E6	1
122	347.1490	3.2	Gibberellin A3			3.9E7	3.8E7	4.7E7	8.0E7	5.8E7	1.0E8	3.1E8	2.1E8	1.2E8	2.1E8	7
100	331.0021	3.2	MEDIA...			4.8E7	5.5E7	5.0E7	8.1E7	6.0E7	8.6E7	1.4E8	3.4E8	7.9E7	2.1E8	1
76	438.2277	3.8	Acromolactone B			6.6E7	1.2E8	5.3E7	8.2E7	6.0E7	1.0E8					
107	622.3646	2.1	MEDIA...			4.5E7	4.0E7	6.1E7	8.5E7	5.7E7	7.8E7	3.1E8	2.2E8	9.0E7	1.5E8	9
112	161.0961	2.9				4.3E7	5.9E7	3.9E7	9.0E7	5.0E7	9.1E7	6.9E7	1.4E8	5.4E7	1.1E8	5

THE PEAKLIST

	m/z	Rt	id	exp1	exp2	exp3	exp4	exp5	exp6	exp7	exp8	exp9	exp10	exp11	exp12
262	343.1541066	3.287420433	3-(1,3,5-Heptatrienyl)-3,4-dihydro-2H-pyran	7755293	7849537	6312070	8.81E+07	9.95E+07	5.37E+07	2.05E+07	2.85E+07	2.42E+07	4.89E+07	3.23E+07	1.00E+08
361	311.3137737	4.922089216		1.68E+07	3.20E+07	1.94E+07	9508327	5.03E+07	9.63E+07	3.88E+07	2.66E+08	3.96E+07	3.05E+07	2.92E+07	1.99E+07
337	329.1383802	3.117513904		1.64E+07	1.88E+07	1.61E+07	3.64E+07	4.05E+07	5.63E+07	4.19E+07	6.28E+07	9550197	1.81E+07	3.34E+07	9.99E+07
256	357.096922	2.450334055	[p-Terphenyl]-2',3,3',3'',4,4'	4977389.5	5769221.5	4035818.3	2.32E+08	5.13E+07	7.16E+07	2.51E+07	1.42E+07	4.88E+08	2.49E+08	8298942.5	1.32E+07
468	375.3046875	4.629094118	Ergosta-2,5,7,9(11),14,22-h	3850456.5	2391488.3	2558098.5	9485285	4.39E+07	1.60E+07	6.05E+07	1.14E+08	1.21E+07	3.38E+07	3568934.3	2.45E+07
492	219.0652425	1.878742576	Inotilone	3.16E+07	3.26E+07	1.70E+07	3478620.8	2.14E+07	3.51E+07	5.88E+07	5.44E+07	7014987.5	1.16E+07	2.69E+07	2.53E+07
271	308.1856555	3.215188054	Cordypyridone D	2.08E+07	1.67E+07	1.38E+07	6.51E+07	9.85E+07	6.31E+07	8.17E+07	9.65E+07	1.27E+07	1.46E+07	2.35E+07	7.51E+07
424	237.0757523	1.876827216	6,8-Dihydroxy-4-(hydroxyn	2.89E+07	2.97E+07	1.60E+07	4608303	2.35E+07	3.51E+07	5.18E+07	5.33E+07	7966711.5	1.19E+07	2.66E+07	2.39E+07
332	173.0961752	2.132396502	4-Dodecene-6,8,10-triyn-3	1.25E+07	9591951	9056542	2.15E+07	4.80E+07	5.20E+07	3.14E+07	3.13E+07	1.56E+07	2.19E+07	3.27E+07	4.25E+07
623	151.0390306	2.935576948	7-Hydroxyphthalide	2.94E+07	3.32E+07	3.83E+07	2.98E+07	5.01E+07	5.26E+07	4.53E+07	4.37E+07	2.54E+07	2.76E+07	4.14E+07	4.25E+07
485	287.1754395	2.717361112	4-(3-Methyl-2-butenyl)tryp	0	0	0	0	0	0	4.75E+07	6.52E+07	0	0	0	0
578	290.1750856	2.884315868		8296270	4690475	5654873.5	1.99E+07	2.73E+07	2.16E+07	2.76E+07	3.97E+07	3200456	3983589	6487381	4.47E+07
287	197.1536722	2.527644591	Dihydro-5-(2-octenyl)-2(3H	3.04E+07	1.39E+07	1.52E+07	3.65E+07	5.17E+07	5.63E+07	3.65E+07	3.98E+07	2.75E+07	2.70E+07	2.92E+07	4.16E+07
266	213.0910335	0.505062745	13-Nor-11-oxo-1(10),2,4,6,	5.74E+07	3.59E+07	1.98E+07	8.32E+07	5.45E+07	6.39E+07	3.07E+07	2.86E+07	1.17E+08	4.57E+07	4.75E+07	2.48E+07
626	372.1806811	3.190111873	3-(4-Hydroxyphenyl)-4-(2-r	2.30E+07	9654425	1.07E+07	3.26E+07	2.21E+07	4.90E+07	5.86E+07	1.27E+08	3879341.8	6874471	1.00E+07	3.97E+07
165	438.2276713	3.845329473	Acremolactone B	5.31E+07	6.58E+07	6.01E+07	0	0	0	0	0	0	0	88571.773	0
619	301.2009726	2.73988587	Achaetolide	1.27E+07	1.47E+07	1.90E+07	1.85E+07	3.04E+07	2.57E+07	1.09E+08	1.92E+08	1.89E+07	3.33E+07	1.92E+07	2.52E+07
195	301.1434766	2.832020789	3-(1,3,5-Heptatrienyl)-3,4-d	3.01E+07	3.68E+07	3.42E+07	3.29E+07	4.37E+07	7.75E+07	3.32E+07	2.51E+07	5.51E+07	9.01E+07	4.74E+07	5.07E+07
327	247.0965599	2.089911343	3,4-Dihydro-6,8-dihydroxy-	5884962.5	5124680	6099616	1.08E+07	5.43E+07	3.94E+07	3.09E+07	3.97E+07	7240481	1.72E+07	2.38E+07	3.41E+07
391	487.2692494	3.43539249	Prasinic acid; O-De-Me	5.65E+07	4.37E+07	2.52E+07	1507433.5	3.77E+07	4.21E+07	1.23E+08	6.83E+07	6809030.5	2.85E+07	3.18E+07	3.62E+07
432	284.1621277	2.937006231	[M+Na-H] 21.9825 m/z add	0	0	0	0	0	0	4.53E+07	4.28E+07	0	0	0	0
501	263.237004	4.636302941		2.41E+07	1.95E+07	1.48E+07	1.84E+07	3.51E+07	2.54E+07	5.00E+07	5.11E+07	2.92E+07	3.22E+07	1.75E+07	2.38E+07
624	356.1856659	3.19104838	Monascopyridine A	1.43E+08	2.12E+08	1.99E+08	310951.97	463368.88	740177.75	615825.19	1411471.9	0	0	322388	560455.25
324	263.0914746	2.168000672	Chaetoatrosin A	1.27E+07	9582966	9591874	2.63E+07	5.68E+07	5.92E+07	3.35E+07	2.30E+07	2.67E+07	4.44E+07	2.43E+07	3.08E+07
443	374.1963205	2.99311225		1.19E+07	7957292.5	7301359	1.61E+07	2.50E+07	2.50E+07	3.81E+07	5.74E+07	2857935.5	3618081.8	7321124.5	4.32E+07
162	837.355249	2.539768205		2.96E+07	8.55E+07	7.22E+07	0	0	0	0	0	0	0	0	0
584	477.3102336	1.972171927		6.29E+07	2.74E+07	3.36E+07	2.03E+07	3.68E+07	3.99E+07	4.23E+07	4.19E+07	1.32E+07	1.59E+07	5.30E+07	3.55E+07
312	309.0968646	2.243265136	Ascolactone A	1.99E+07	1.86E+07	1.93E+07	3.01E+07	7.15E+07	4.35E+07	4.14E+07	3.92E+07	2.71E+07	3.61E+07	2.72E+07	4.02E+07
274	257.1722592	2.194236404	[M+Na-H] 21.9825 m/z add	1.51E+07	7075811	7186897.5	6.08E+07	5.18E+07	3.75E+07	2.03E+07	2.65E+07	4.60E+07	5.71E+07	2.17E+07	4.06E+07
643	407.2177555	3.137295595		2.48E+07	1.24E+07	1.16E+07	2.90E+07	1.94E+07	4.28E+07	4.04E+07	9.40E+07	3956534.3	9582998	1.31E+07	3.61E+07
421	288.1789594	2.784753791		0	175060.47	0	0	0	0	5.57E+07	7.60E+07	0	95759.094	0	0
469	374.3030413	4.409591176		4748985.5	1.29E+07	8323346.5	1.07E+07	3.05E+07	4.15E+07	1.95E+07	1.10E+08	6228114	1.19E+07	1.83E+07	1.82E+07
513	221.1172759	3.060349014	Sohirnone A	3.00E+07	1.89E+07	2.34E+07	1.89E+07	3.56E+07	3.24E+07	3.48E+07	4.28E+07	1.85E+07	2.39E+07	3.41E+07	3.33E+07
272	323.1853638	3.278672806	Zearalenone; (S)-form, 11,	4199147	2434221	2248077	6.44E+07	5.60E+07	4.04E+07	1.71E+07	1.17E+07	1.75E+08	1.15E+08	8810807	8544181
330	259.1693492	2.814300048	5-Hydroxy-2,7-dimethyl-2-	2.39E+07	9781892	1.11E+07	2.99E+07	5.18E+07	5.59E+07	1.94E+07	1.91E+07	1.15E+07	1.51E+07	1.75E+07	4.73E+07
417	624.266571	2.514141098		3.73E+07	1.41E+07	1.82E+07	4990229.5	1.99E+07	4.63E+07	6.17E+07	3.82E+07	1467181.6	4664460.5	1.72E+07	5.23E+07
681	459.3106025	4.61080098	Ergokonin B	7696646.5	5097993.5	6487114	8023549	3.48E+07	1.70E+07	4.44E+07	7.00E+07	8308916.5	1.48E+07	7021781	1.62E+07
673	654.3320887	4.659747059		1.51E+07	2.30E+07	1.45E+07	4873988.5	9729128	2.62E+07	2.93E+07	2.97E+07	4579606	6284409.5	2.17E+07	1.59E+07
86	586.2298315	2.667653049		6.43E+07	3.63E+07	4.81E+07	4949733	8630320	4.21E+07	2.35E+07	1.05E+07	5143420.5	1.95E+07	2.82E+07	3.06E+07
536	263.0550501	1.851977049	Cerdarin; 1-O-De-Me	1.89E+07	7785098	5009049.5	1.69E+08	2.40E+07	7822705	5561140.5	4491372	3.25E+08	1.20E+08	4273709.5	4718831
420	239.1641675	3.067175213	Eujavanoic acid B	6443053	1.08E+07	1.21E+07	1.08E+07	2.59E+07	1.42E+07	5.70E+07	1.00E+08	9694656	1.95E+07	1.15E+07	1.29E+07

Dereplication and statistics : identifying the compounds of interest

262	343.1541066	3.287420433	3-(1,3,5-Heptatrienyl)-3,4-	7755293	7849537	6312070	8.81E+07	9.95E+07	5.37E+07	2.05E+07	2.85E+07	2.42E+07	4.89E+07	3.23E+07	1.00E+08
361	311.3137737	4.922089216		1.68E+07	3.20E+07	1.94E+07	9508327	5.03E+07	9.63E+07	3.88E+07	2.66E+08	3.96E+07	3.05E+07	2.92E+07	1.99E+07
337	329.1383802	3.117513904		1.64E+07	1.88E+07	1.61E+07	3.64E+07	4.05E+07	5.63E+07	4.19E+07	6.28E+07	9550197	1.81E+07	3.34E+07	9.99E+07
256	357.096922	2.450334055	[p-Terphenyl]-2',3',3'',4,4'	977389.5	5769221.5	4035818.3	2.32E+08	5.13E+07	7.16E+07	2.51E+07	1.42E+07	4.88E+08	2.49E+08	8298942.5	1.32E+07
468	375.3046875	4.629094118	Ergosta-2,5,7,9(11),14,22-H	850456.5	2391488.3	2558098.5	9485285	4.39E+07	1.60E+07	6.05E+07	1.14E+08	1.21E+07	3.38E+07	3568934.3	2.45E+07
492	219.0652425	1.878742576	Inotilone	3.16E+07	3.26E+07	1.70E+07	3478620.8	2.14E+07	3.51E+07	5.88E+07	5.44E+07	7014987.5	1.16E+07	2.69E+07	2.53E+07
271	308.1856555	3.215188054	Cordypyridone D	2.08E+07	1.67E+07	1.38E+07	6.51E+07	9.85E+07	6.31E+07	8.17E+07	9.65E+07	1.27E+07	1.46E+07	2.35E+07	7.51E+07
424	237.0757523	1.876827216	6,8-Dihydroxy-4-(hydroxyn	2.89E+07	2.97E+07	1.60E+07	4608303	2.35E+07	3.51E+07	5.18E+07	5.33E+07	7966711.5	1.19E+07	2.66E+07	2.39E+07
332	173.0961752	2.132396502	4-Dodecene-6,8,10-triyn-3	1.25E+07	9591951	9056542	2.15E+07	4.80E+07	5.20E+07	3.14E+07	3.13E+07	1.56E+07	2.19E+07	3.27E+07	4.25E+07
623	151.0390306	2.935576948	7-Hydroxyphthalide	2.94E+07	3.32E+07	3.83E+07	2.98E+07	5.01E+07	5.26E+07	4.53E+07	4.37E+07	2.54E+07	2.76E+07	4.14E+07	4.25E+07
485	287.1754395	2.717361112	4-(3-Methyl-2-butenyl)tryp	0	0	0	0	0	0	4.75E+07	6.52E+07	0	0	0	0
578	290.1750856	2.884315868		8296270	4690475	5654873.5	1.99E+07	2.73E+07	2.16E+07	2.76E+07	3.97E+07	3200456	3983589	6487381	4.47E+07
287	197.1536722	2.527644591	Dihydro-5-(2-octenyl)-2(3H	3.04E+07	1.39E+07	1.52E+07	3.65E+07	5.17E+07	5.63E+07	3.65E+07	3.98E+07	2.75E+07	2.70E+07	2.92E+07	4.16E+07
266	213.0910335	0.505062745	13-Nor-11-oxo-1(10),2,4,6,	5.74E+07	3.59E+07	1.98E+07	8.32E+07	5.45E+07	6.39E+07	3.07E+07	2.86E+07	1.17E+08	4.57E+07	4.75E+07	2.48E+07
626	372.1806811	3.190111873	3-(4-Hydroxyphenyl)-4-(2-r	2.30E+07	9654425	1.07E+07	3.26E+07	2.21E+07	4.90E+07	5.86E+07	1.27E+08	3879341.8	6874471	1.00E+07	3.97E+07
165	438.2276713	3.845329473	Acremolactone B	5.31E+07	6.58E+07	6.01E+07	0	0	0	0	0	0	0	88571.773	0
619	301.2009726	2.73988587	Achaetolide	1.27E+07	1.47E+07	1.90E+07	1.85E+07	3.04E+07	2.57E+07	1.09E+08	1.92E+08	1.89E+07	3.33E+07	1.92E+07	2.52E+07
195	301.1434766	2.832020789	3-(1,3,5-Heptatrienyl)-3,4-	3.01E+07	3.68E+07	3.42E+07	3.29E+07	4.37E+07	7.75E+07	3.32E+07	2.51E+07	5.51E+07	9.01E+07	4.74E+07	5.07E+07
327	247.0965599	2.089911343	3,4-Dihydro-6,8-dihydroxy-	884962.5	5124680	6099616	1.08E+07	5.43E+07	3.94E+07	3.09E+07	3.97E+07	7240481	1.72E+07	2.38E+07	3.41E+07
391	487.2692494	3.43539249	Prasinic acid; O-De-Me	5.65E+07	4.37E+07	2.52E+07	1507433.5	3.77E+07	4.21E+07	1.23E+08	6.83E+07	6809030.5	2.85E+07	3.18E+07	3.62E+07
432	284.1621277	2.937006231	[M+Na-H] 21.9825 m/z add	0	0	0	0	0	0	4.53E+07	4.28E+07	0	0	0	0
501	263.237004	4.636302941		2.41E+07	1.95E+07	1.48E+07	1.84E+07	3.51E+07	2.54E+07	5.00E+07	5.11E+07	2.92E+07	3.22E+07	1.75E+07	2.38E+07
624	356.1856659	3.19104838	Monascopyridine A	1.43E+08	2.12E+08	1.99E+08	310951.97	463368.88	740177.75	615825.19	1411471.9	0	0	322388	560455.25
324	263.0914746	2.168000672	Chaetoatrosin A	1.27E+07	9582966	9591874	2.63E+07	5.68E+07	5.92E+07	3.35E+07	2.30E+07	2.67E+07	4.44E+07	2.43E+07	3.08E+07
443	374.1963205	2.99311225		1.19E+07	7957292.5	7301359	1.61E+07	2.50E+07	2.50E+07	3.81E+07	5.74E+07	2857935.5	3618081.8	7321124.5	4.32E+07
162	837.355249	2.539768205		2.96E+07	8.55E+07	7.22E+07	0	0	0	0	0	0	0	0	0
584	477.3102336	1.972171927		6.29E+07	2.74E+07	3.36E+07	2.03E+07	3.68E+07	3.99E+07	4.23E+07	4.19E+07	1.32E+07	1.59E+07	5.30E+07	3.55E+07
312	309.0968646	2.243265136	Ascolactone A	1.99E+07	1.86E+07	1.93E+07	3.01E+07	7.15E+07	4.35E+07	4.14E+07	3.92E+07	2.71E+07	3.61E+07	2.72E+07	4.02E+07
274	257.1722592	2.194236404	[M+Na-H] 21.9825 m/z add	1.51E+07	7075811	7186897.5	6.08E+07	5.18E+07	3.75E+07	2.03E+07	2.65E+07	4.60E+07	5.71E+07	2.17E+07	4.06E+07
643	407.2177555	3.137295595		2.48E+07	1.24E+07	1.16E+07	2.90E+07	1.94E+07	4.28E+07	4.04E+07	9.40E+07	3956534.3	9582998	1.31E+07	3.61E+07
421	288.1789594	2.784753791		0	175060.47	0	0	0	0	5.57E+07	7.60E+07	0	95759.094	0	0
469	374.3030413	4.409591176		748985.5	1.29E+07	8323346.5	1.07E+07	3.05E+07	4.15E+07	1.95E+07	1.10E+08	6228114	1.19E+07	1.83E+07	1.82E+07
513	221.1172759	3.060349014	Sohirnone A	3.00E+07	1.89E+07	2.34E+07	1.89E+07	3.56E+07	3.24E+07	3.48E+07	4.28E+07	1.85E+07	2.39E+07	3.41E+07	3.33E+07
272	323.1853638	3.278672806	Zearalenone; (S)-form, 11,	4199147	2434221	2248077	6.44E+07	5.60E+07	4.04E+07	1.71E+07	1.17E+07	1.75E+08	1.15E+08	8810807	8544181
330	259.1693492	2.814300048	5-Hydroxy-2,7-dimethyl-2-	2.39E+07	9781892	1.11E+07	2.99E+07	5.18E+07	5.59E+07	1.94E+07	1.91E+07	1.15E+07	1.51E+07	1.75E+07	4.73E+07
417	624.266571	2.514141098		3.73E+07	1.41E+07	1.82E+07	4990229.5	1.99E+07	4.63E+07	6.17E+07	3.82E+07	1467181.6	4664460.5	1.72E+07	5.23E+07
681	459.3106025	4.61080098	Ergokonin B	696646.5	5097993.5	6487114	8023549	3.48E+07	1.70E+07	4.44E+07	7.00E+07	8308916.5	1.48E+07	7021781	1.62E+07
673	654.3320887	4.659747059		1.51E+07	2.30E+07	1.45E+07	4873988.5	9729128	2.62E+07	2.93E+07	2.97E+07	4579606	6284409.5	2.17E+07	1.59E+07
86	586.2298315	2.667653049		6.43E+07	3.63E+07	4.81E+07	4949733	8630320	4.21E+07	2.35E+07	1.05E+07	5143420.5	1.95E+07	2.82E+07	3.06E+07
536	263.0550501	1.851977049	Cerdarin; 1-O-De-Me	1.89E+07	7785098	5009049.5	1.69E+08	2.40E+07	7822705	5561140.5	4491372	3.25E+08	1.20E+08	4273709.5	4718831
420	239.1641675	3.067175213	Eujavanoic acid B	6443053	1.08E+07	1.21E+07	1.08E+07	2.59E+07	1.42E+07	5.70E+07	1.00E+08	9694656	1.95E+07	1.15E+07	1.29E+07

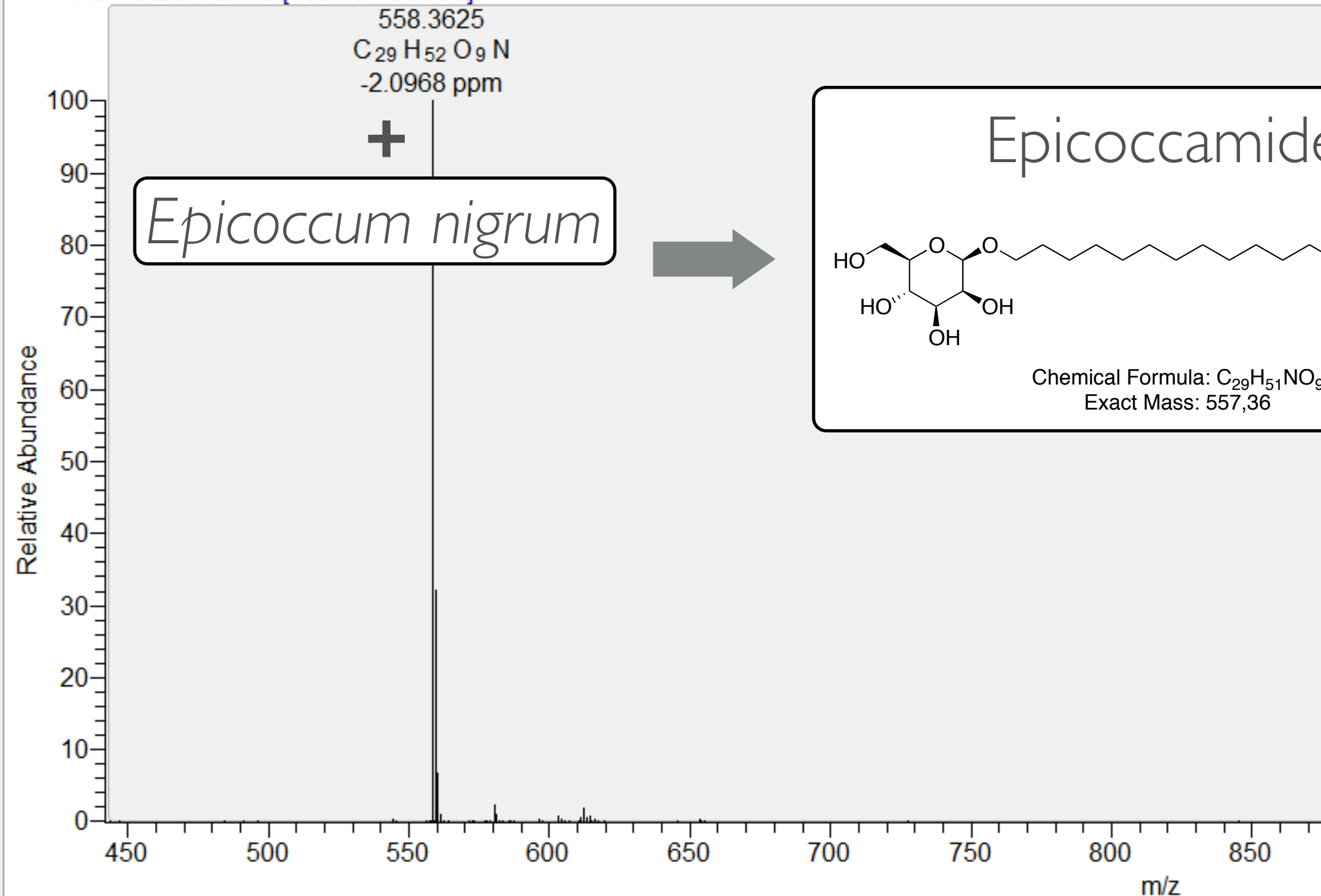


OPLS-DA model
CV-ANOVA p < 5%

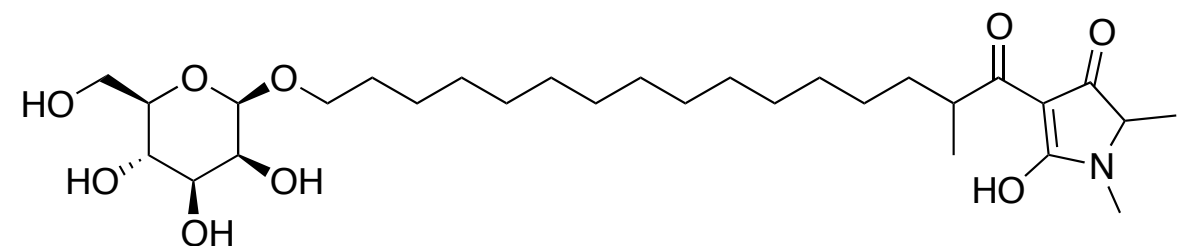


Natural Products DB (3ppm tol)

20140112_PMA_PMA1_7_35_SPE_pos #883 RT: 3.87 AV: 1 NL: 1.72E9
T: FTMS + c ESI Full ms [150.00-1300.00]

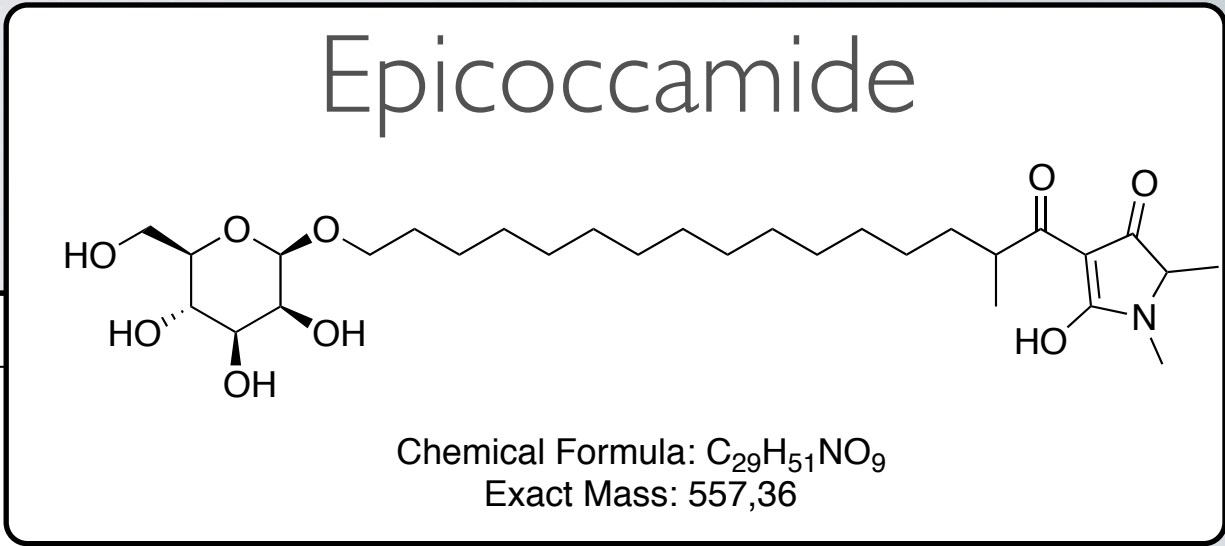


Epicoccamide

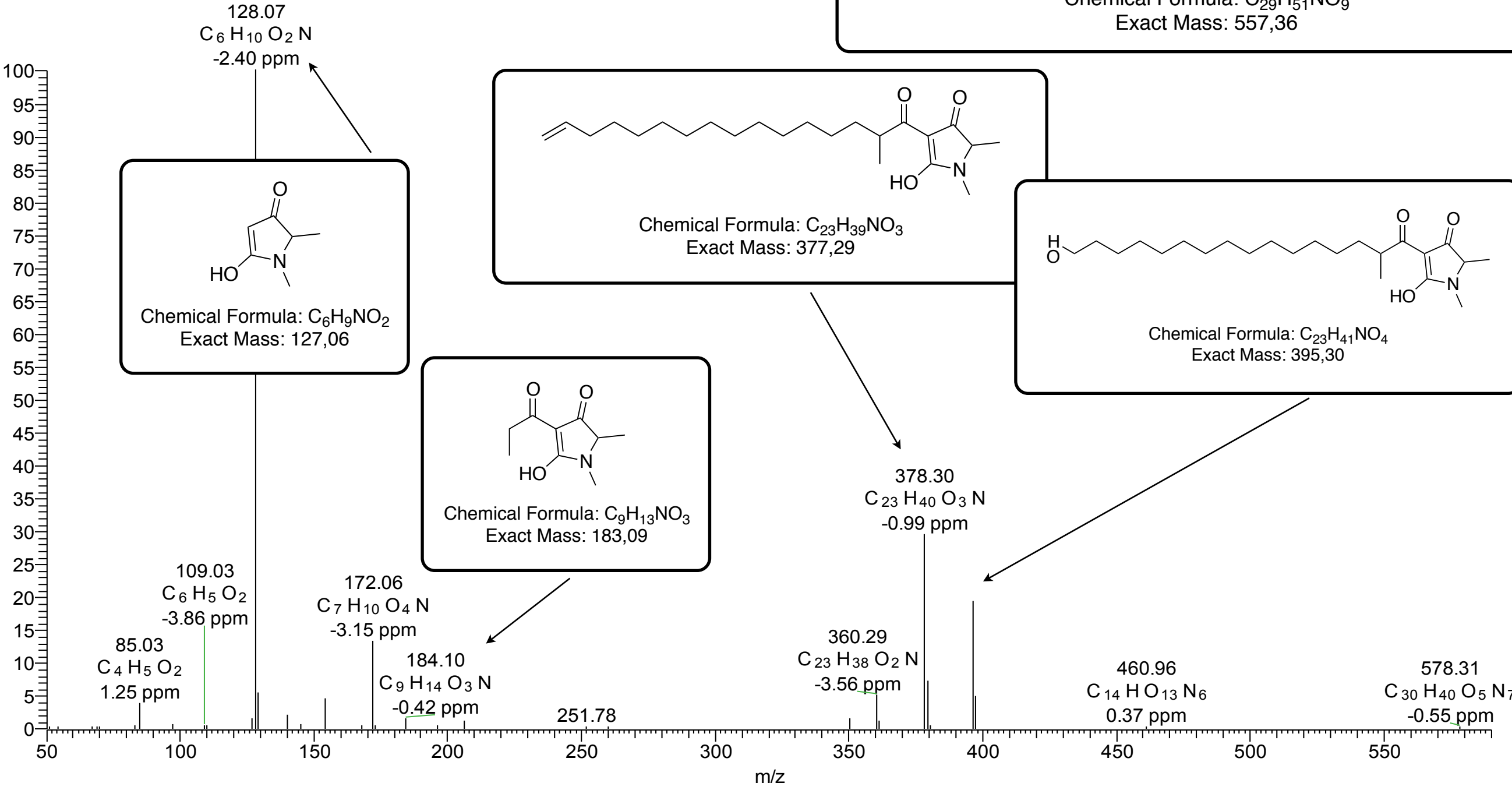


Chemical Formula: $C_{29}H_{51}NO_9$
Exact Mass: 557,36

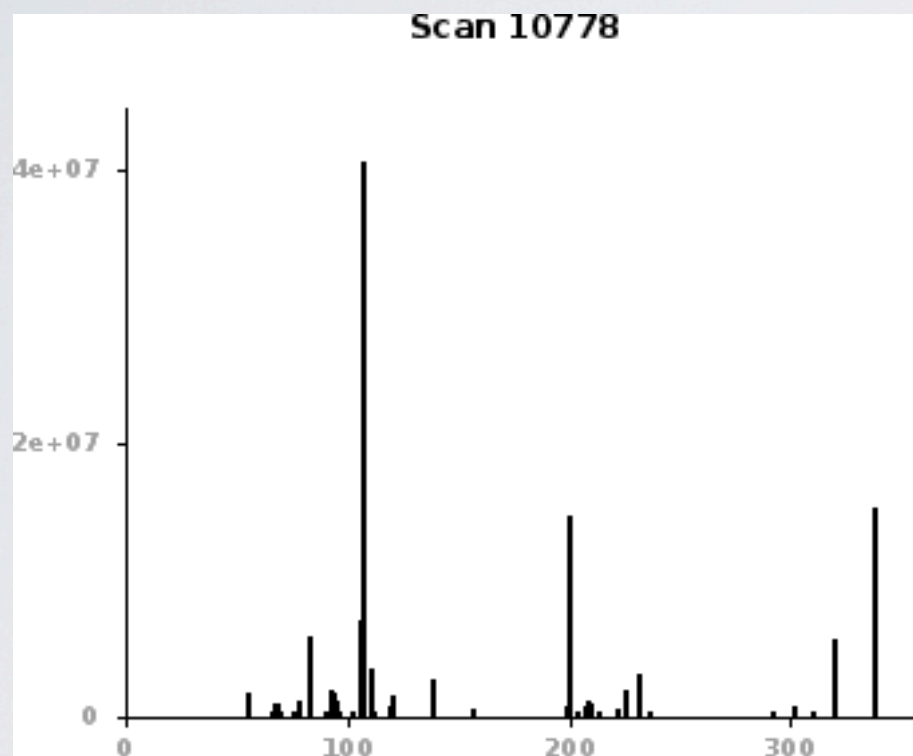
MS² level : fragments give structural information



131128_PMA_PMA1_3_5_pos_70000_FullMS_... 17/03/2013 16:29:47
131128_PMA_PMA1_3_5_pos_70000_FullMS_ddMS2_Top1 #2238 RT: 3.89 AV: 1 NL: 8.87E7
T: FTMS + c ESI d Full ms2 558.36@hcd30.00 [50.00-590.00]



Molecular barcodes



$\approx$



Many molecular barcodes, very informative, but ...
($\approx$ 10000 MS2 scans in a 10 min run)



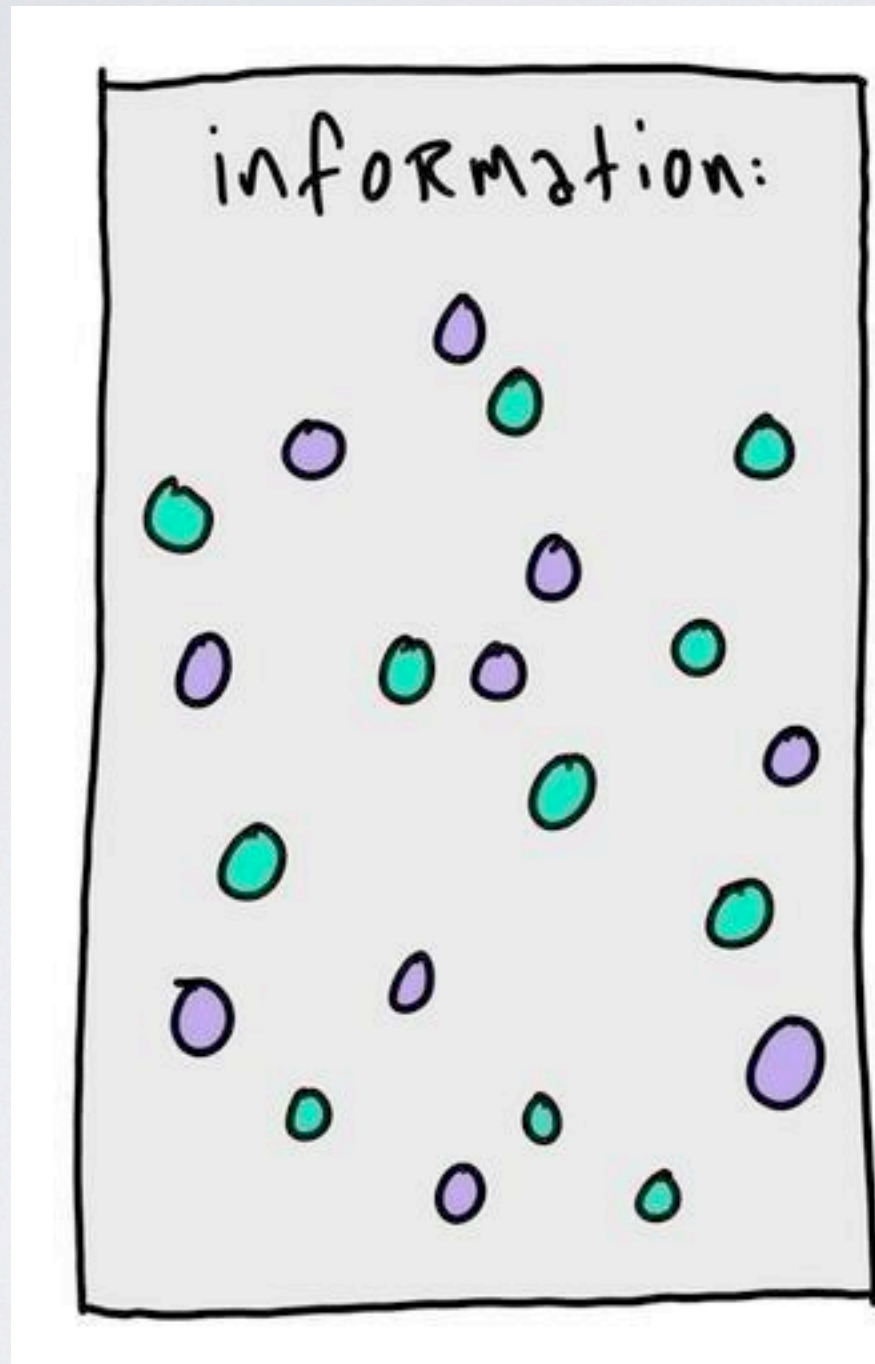
Information overload



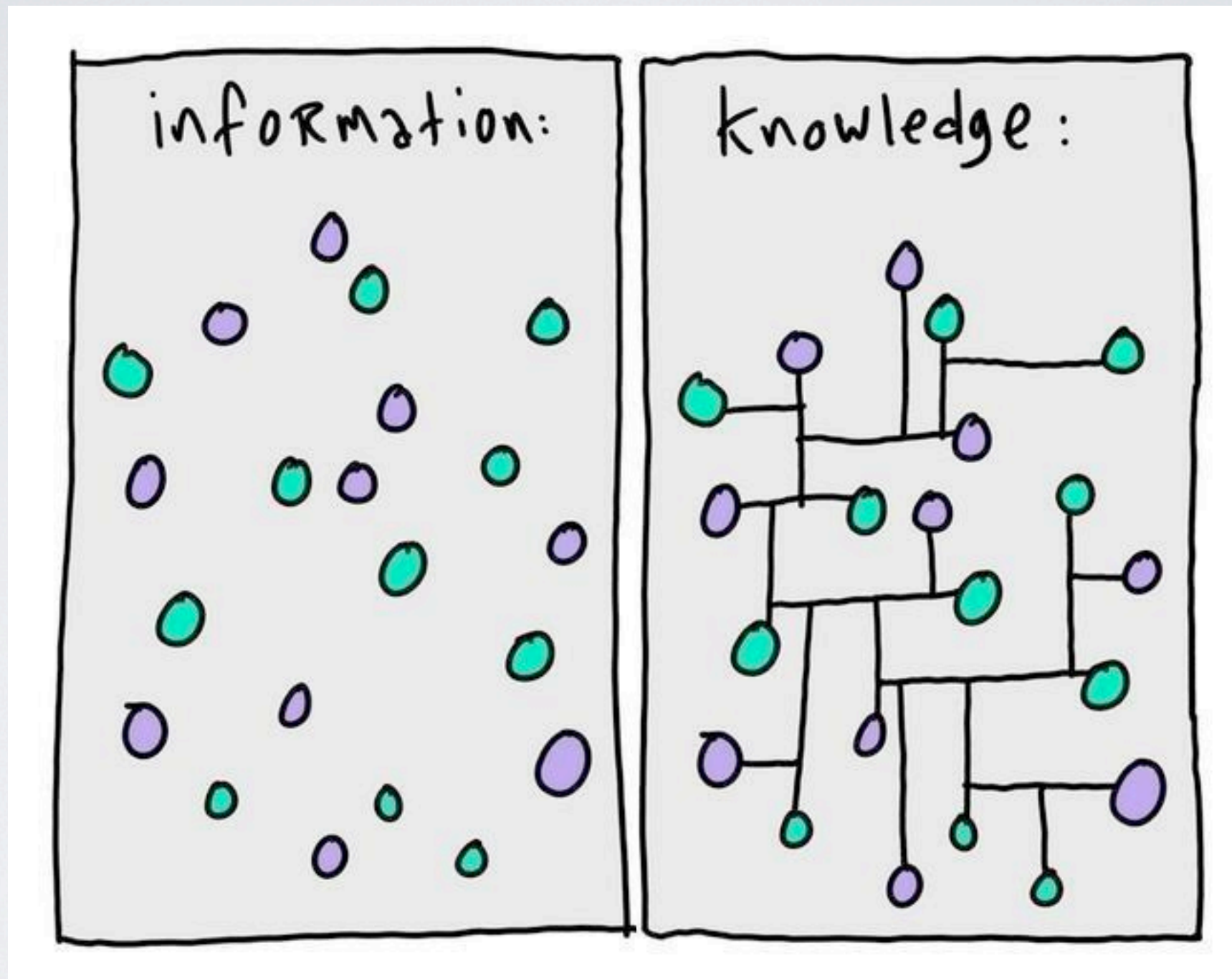
What is information ?



MS² data : from information to knowledge



MS² data : from information to knowledge

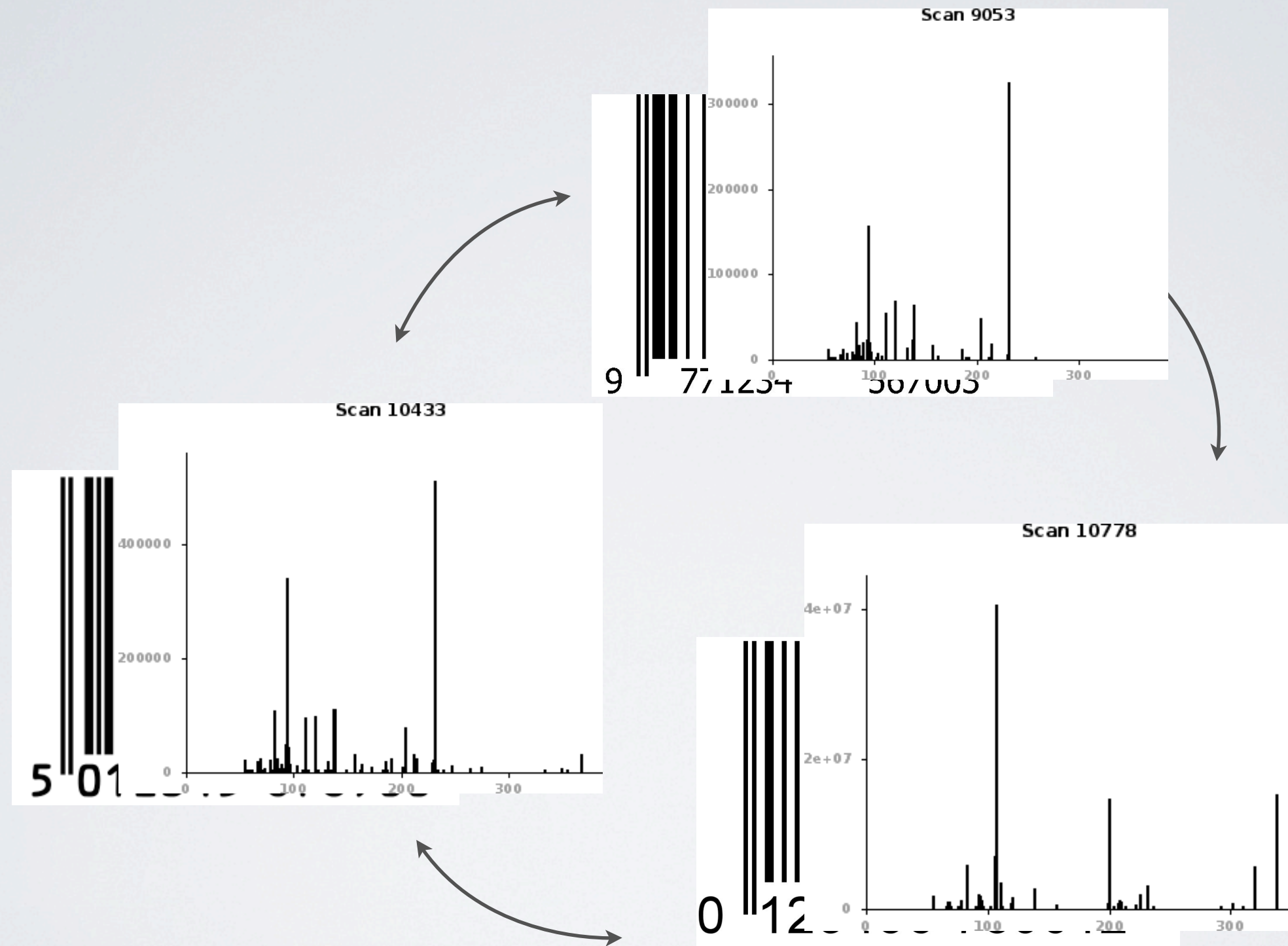


Spectral Networks package - UCSD Bioinformatics



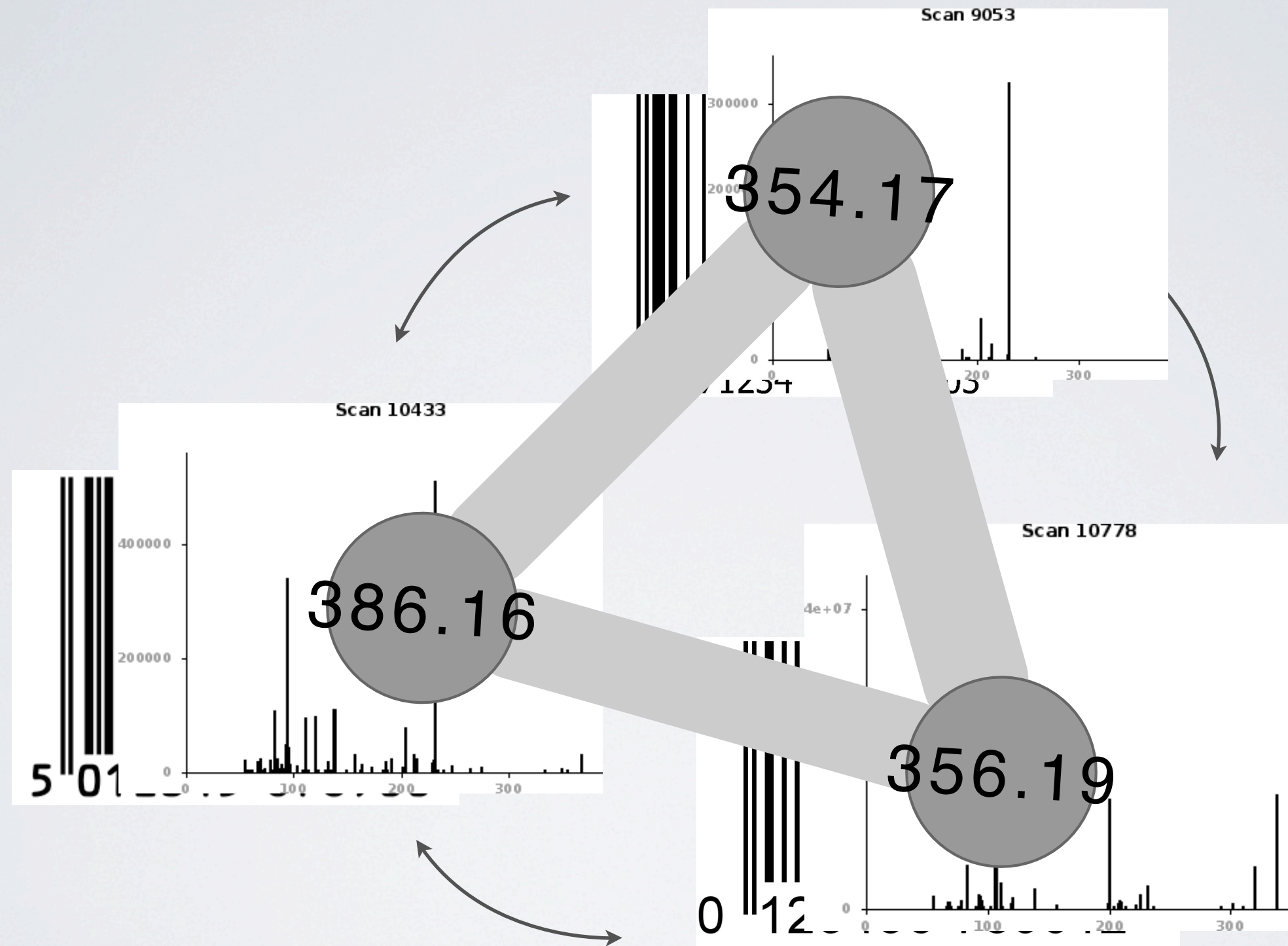
J. Watrous et al. "Mass spectral molecular networking of living microbial colonies," *PNAS*, vol. 109, no. 26, pp. E1743–52, **2012**.

Spectral Networks package - UCSD Bioinformatics



J. Watrous et al. "Mass spectral molecular networking of living microbial colonies," *PNAS*, vol. 109, no. 26, pp. E1743–52, **2012**.

Spectral Networks package - UCSD Bioinformatics

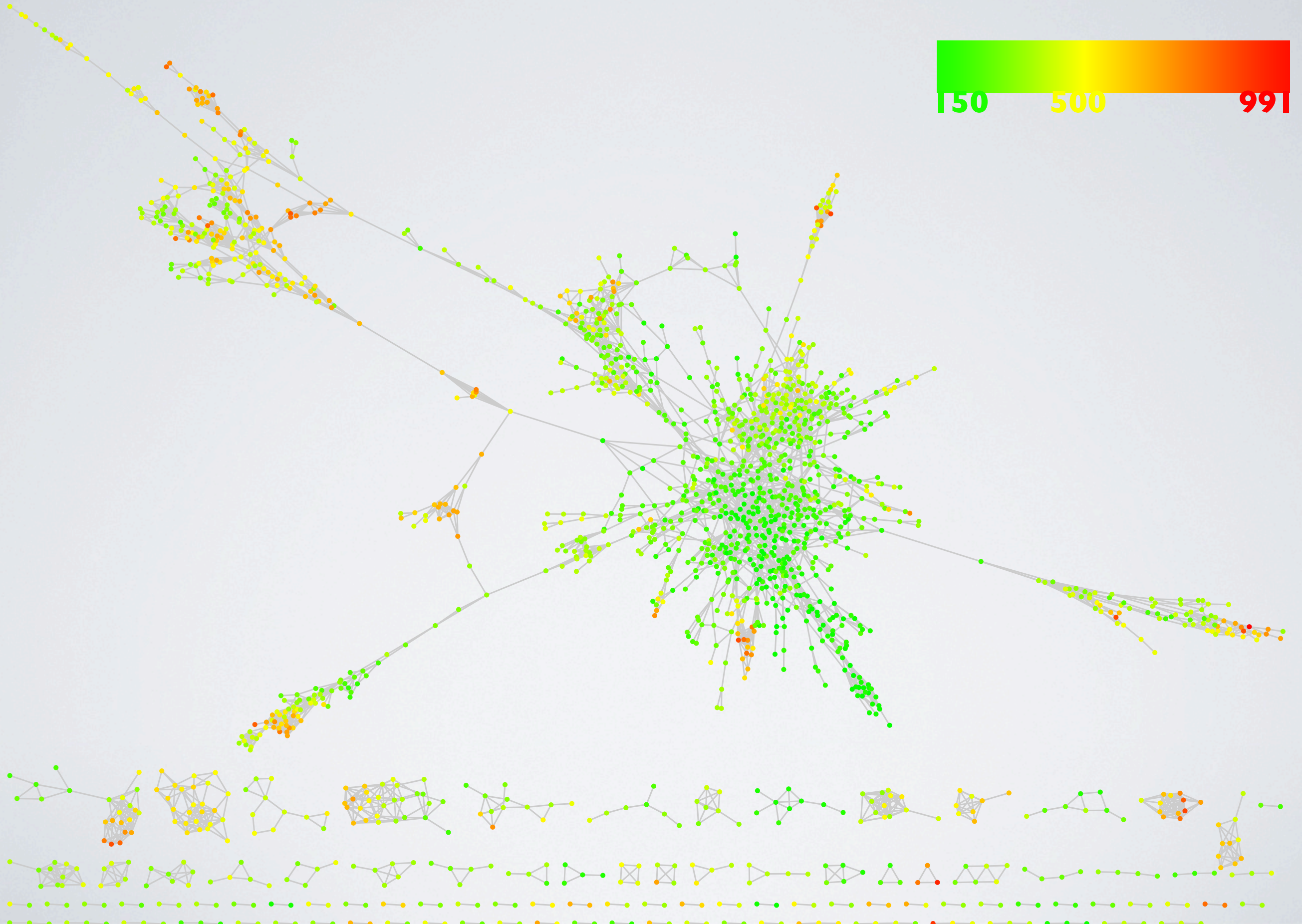


J. Watrous et al. "Mass spectral molecular networking of living microbial colonies," *PNAS*, vol. 109, no. 26, pp. E1743–52, **2012**.

Molecular networks

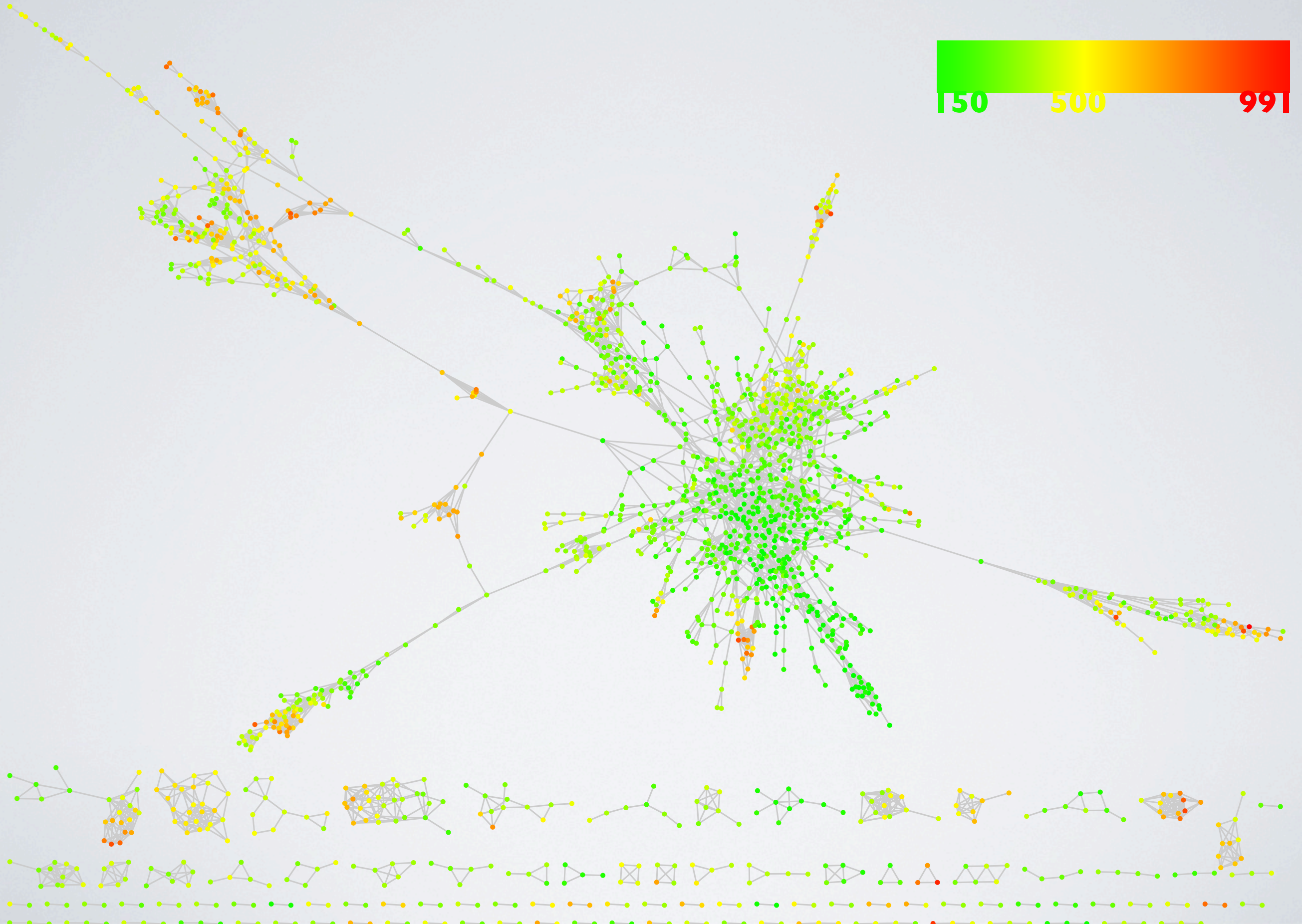


Molecular networks



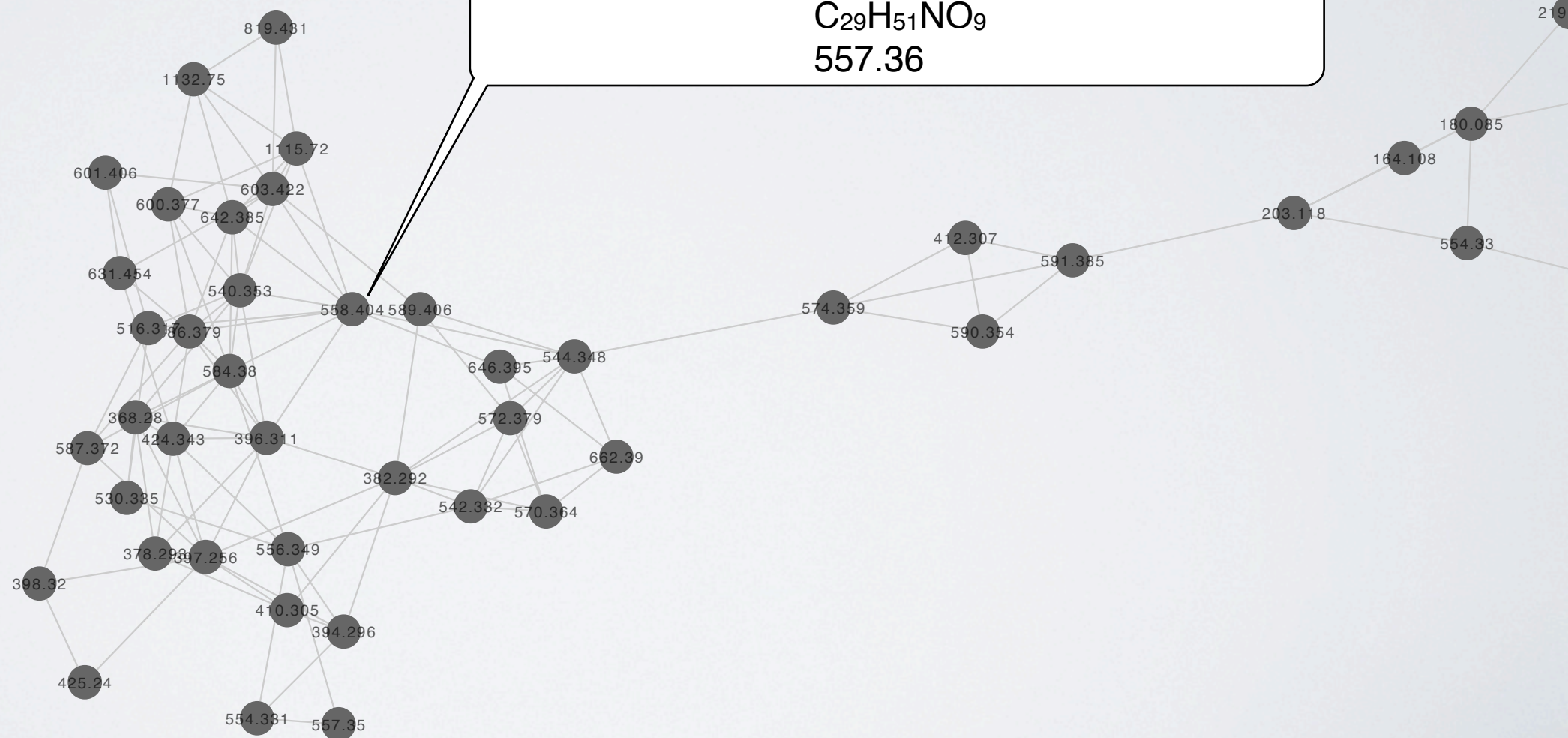
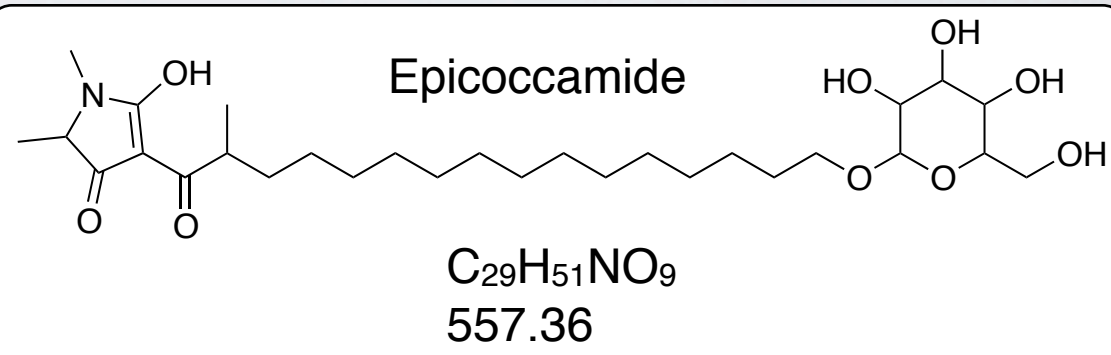
262	343.1541066	3.287420433	3-(1,3,5-Heptatrienyl)-3,4-d	7755293	7849537	6312070	8.81E+07	9.95E+07	5.37E+07	2.05E+07	2.85E+07	2.42E+07	4.89E+07	3.23E+07	1.00E+08	5.62E+07	3.88E+07	7.07E+07	6.59E+07	4.36E+07
361	311.3137737	4.922089216		1.68E+07	3.20E+07	1.94E+07	9508327	5.03E+07	9.63E+07	3.88E+07	2.66E+08	3.96E+07	3.05E+07	2.92E+07	1.99E+07	1.79E+08	6.93E+07	1.36E+07	1.02E+08	7.11E+07
337	329.1383802	3.117513904		1.64E+07	1.88E+07	1.61E+07	3.64E+07	4.05E+07	5.63E+07	4.19E+07	6.28E+07	9550197	1.81E+07	3.34E+07	9.99E+07	6.62E+07	4.62E+07	7.73E+07	8.31E+07	5.18E+07
256	357.096922	2.450334055	[p-Terphenyl]-2',3,3',3'',4,4'	4977389.5	5769221.5	4035818.3	2.32E+08	5.13E+07	7.16E+07	2.51E+07	1.42E+07	4.88E+08	2.49E+08	8298942.5	1.32E+07	2.77E+07	6.63E+07	5.86E+07	1.93E+07	6.80E+07
468	375.3046875	4.629094118	Ergosta-2,5,7,9(11),14,22-t	3850456.5	2391488.3	2558098.5	9485285	4.39E+07	1.60E+07	6.05E+07	1.14E+08	1.21E+07	3.38E+07	3568934.3	2.45E+07	5.60E+07	3.46E+07	4.72E+07	1.81E+08	4.01E+07
492	219.0652425	1.878742576	Inotilone	3.16E+07	3.26E+07	1.70E+07	3478620.8	2.14E+07	3.51E+07	5.88E+07	5.44E+07	7014987.5	1.16E+07	2.69E+07	2.53E+07	2.33E+07	3.62E+07	3.25E+07	9.70E+07	3.86E+07
271	308.1856555	3.215188054	Cordypyridone D	2.08E+07	1.67E+07	1.38E+07	6.51E+07	9.85E+07	6.31E+07	8.17E+07	9.65E+07	1.27E+07	1.46E+07	2.35E+07	7.51E+07	4.82E+07	4.63E+07	1.15E+08	1.39E+08	7.95E+07
424	237.0757523	1.876827216	6,8-Dihydroxy-4-(hydroxyn	2.89E+07	2.97E+07	1.60E+07	4608303	2.35E+07	3.51E+07	5.18E+07	5.33E+07	7966711.5	1.19E+07	2.66E+07	2.39E+07	2.57E+07	3.40E+07	3.50E+07	9.12E+07	3.89E+07
332	173.0961752	2.132396502	4-Dodecene-6,8,10-triyn-3	1.25E+07	9591951	9056542	2.15E+07	4.80E+07	5.20E+07	3.14E+07	3.13E+07	1.56E+07	2.19E+07	3.27E+07	4.25E+07	4.24E+07	2.78E+07	5.90E+07	5.16E+07	2.49E+07
623	151.0390306	2.935576948	7-Hydroxyphthalide	2.94E+07	3.32E+07	3.83E+07	2.98E+07	5.01E+07	5.26E+07	4.53E+07	4.37E+07	2.54E+07	2.76E+07	4.14E+07	4.25E+07	4.79E+07	4.09E+07	5.02E+07	5.19E+07	3.97E+07
485	287.1754395	2.717361112	4-(3-Methyl-2-butenyl)tryp	0	0	0	0	0	0	4.75E+07	6.52E+07	0	0	0	0	0	1.55E+07	0	6.69E+07	1.53E+07
578	290.1750856	2.884315868		8296270	4690475	5654873.5	1.99E+07	2.73E+07	2.16E+07	2.76E+07	3.97E+07	3200456	3983589	6487381	4.47E+07	2.35E+07	2.58E+07	5.57E+07	7.05E+07	2.84E+07
287	197.1536722	2.527644591	Dihydro-5-(2-octenyl)-2(3H	3.04E+07	1.39E+07	1.52E+07	3.65E+07	5.17E+07	5.63E+07	3.65E+07	3.98E+07	2.75E+07	2.70E+07	2.92E+07	4.16E+07	3.98E+07	3.70E+07	4.09E+07	6.06E+07	3.59E+07
266	213.0910335	0.505062745	13-Nor-11-oxo-1(10),2,4,6,	5.74E+07	3.59E+07	1.98E+07	8.32E+07	5.45E+07	6.39E+07	3.07E+07	2.86E+07	1.17E+08	4.57E+07	4.75E+07	2.48E+07	2.55E+07	7.04E+07	9.37E+07	4.35E+07	4.42E+07
626	372.1806811	3.190111873	3-(4-Hydroxyphenyl)-4-(2-r	2.30E+07	9654425	1.07E+07	3.26E+07	2.21E+07	4.90E+07	5.86E+07	1.27E+08	3879341.8	6874471	1.00E+07	3.97E+07	1.93E+07	3.70E+07	8.67E+07	1.01E+08	3.92E+07
165	438.2276713	3.845329473	Acremolactone B	5.31E+07	6.58E+07	6.01E+07	0	0	0	0	0	0	0	88571.773	0	0	1.23E+07	0	0	1.22E+07
619	301.2009726	2.73988587	Achaetolide	1.27E+07	1.47E+07	1.90E+07	1.85E+07	3.04E+07	2.57E+07	1.09E+08	1.92E+08	1.89E+07	3.33E+07	1.92E+07	2.52E+07	2.81E+07	4.85E+07	2.95E+07	1.83E+08	5.80E+07
195	301.1434766	2.832020789	3-(1,3,5-Heptatrienyl)-3,4-t	3.01E+07	3.68E+07	3.42E+07	3.29E+07	4.37E+07	7.75E+07	3.32E+07	2.51E+07	5.51E+07	9.01E+07	4.74E+07	5.07E+07	8.87E+07	4.49E+07	4.92E+07	2.51E+07	4.61E+07
327	247.0965599	2.089911343	3,4-Dihydro-6,8-dihydroxy-	5884962.5	5124680	6099616	1.08E+07	5.43E+07	3.94E+07	3.09E+07	3.97E+07	7240481	1.72E+07	2.38E+07	3.41E+07	1.20E+08	2.92E+07	4.03E+07	5.44E+07	2.76E+07
391	487.2692494	3.43539249	Prasinic acid; O-De-Me	5.65E+07	4.37E+07	2.52E+07	1507433.5	3.77E+07	4.21E+07	1.23E+08	6.83E+07	6809030.5	2.85E+07	3.18E+07	3.62E+07	1.75E+07	4.53E+07	1.66E+07	7.91E+07	3.78E+07
432	284.1621277	2.937006231	[M+Na-H] 21.9825 m/z adc	0	0	0	0	0	0	4.53E+07	4.28E+07	0	0	0	0	0	1.58E+07	0	4.59E+07	1.60E+07
501	263.237004	4.636302941		2.41E+07	1.95E+07	1.48E+07	1.84E+07	3.51E+07	2.54E+07	5.00E+07	5.11E+07	2.92E+07	3.22E+07	1.75E+07	2.38E+07	3.67E+07	3.03E+07	3.46E+07	6.75E+07	2.64E+07
624	356.1856659	3.19104838	Monascopyridine A	1.43E+08	2.12E+08	1.99E+08	310951.97	463368.88	740177.75	615825.19	1411471.9	0	0	322388	560455.25	436921.97	3.87E+07	826371.75	1282738.9	4.21E+07
324	263.0914746	2.168000672	Chaetoatrosin A	1.27E+07	9582966	9591874	2.63E+07	5.68E+07	5.92E+07	3.35E+07	2.30E+07	2.67E+07	4.44E+07	2.43E+07	3.08E+07	4.42E+07	3.16E+07	4.33E+07	2.44E+07	3.07E+07
443	374.1963205	2.99311225		1.19E+07	7957292.5	7301359	1.61E+07	2.50E+07	2.50E+07	3.81E+07	5.74E+07	2857935.5	3618081.8	7321124.5	4.32E+07	2.48E+07	2.90E+07	5.54E+07	6.43E+07	2.56E+07
162	837.355249	2.539768205		2.96E+07	8.55E+07	7.22E+07	0	0	0	0	0	0	0	0	0	0	4056636.5	0	0	4369688.5
584	477.3102336	1.972171927		6.29E+07	2.74E+07	3.36E+07	2.03E+07	3.68E+07	3.99E+07	4.23E+07	4.19E+07	1.32E+07	1.59E+07	5.30E+07	3.55E+07	3.41E+07	4.24E+07	4.95E+07	8.44E+07	3.90E+07
312	309.0968646	2.243265136	Ascolactone A	1.99E+07	1.86E+07	1.93E+07	3.01E+07	7.15E+07	4.35E+07	4.14E+07	3.92E+07	2.71E+07	3.61E+07	2.72E+07	4.02E+07	5.03E+07	3.53E+07	4.66E+07	4.81E+07	3.79E+07
274	257.1722592	2.194236404	[M+Na-H] 21.9825 m/z adc	1.51E+07	7075811	7186897.5	6.08E+07	5.18E+07	3.75E+07	2.03E+07	2.65E+07	4.60E+07	5.71E+07	2.17E+07	4.06E+07	3.21E+07	2.28E+07	2.63E+07	2.55E+07	2.23E+07
643	407.2177555	3.137295595		2.48E+07	1.24E+07	1.16E+07	2.90E+07	1.94E+07	4.28E+07	4.04E+07	9.40E+07	3956534.3	9582998	1.31E+07	3.61E+07	1.71E+07	4.07E+07	5.49E+07	4.74E+07	4.01E+07
421	288.1789594	2.784753791		0	175060.47	0	0	0	0	5.57E+07	7.60E+07	0	95759.094	0	0	0	1.59E+07	0	7.85E+07	1.81E+07
469	374.3030413	4.409591176		4748985.5	1.29E+07	8323346.5	1.07E+07	3.05E+07	4.15E+07	1.95E+07	1.10E+08	6228114	1.19E+07	1.83E+07	1.82E+07	3.08E+07	2.79E+07	1.06E+07	2.31E+07	2.15E+07
513	221.1172759	3.060349014	Sohirnone A	3.00E+07	1.89E+07	2.34E+07	1.89E+07	3.56E+07	3.24E+07	3.48E+07	4.28E+07	1.85E+07	2.39E+07	3.41E+07	3.33E+07	4.20E+07	3.57E+07	3.81E+07	6.00E+07	3.31E+07
272	323.1853638	3.278672806	Zearalenone; (S)-form, 11,	4199147	2434221	2248077	6.44E+07	5.60E+07	4.04E+07	1.71E+07	1.17E+07	1.75E+08	1.15E+08	8810807	8544181	2.74E+07	3.21E+07	1.45E+07	1.64E+07	3.45E+07
330	259.1693492	2.814300048	5-Hydroxy-2,7-dimethyl-2-	2.39E+07	9781892	1.11E+07	2.99E+07	5.18E+07	5.59E+07	1.94E+07	1.91E+07	1.15E+07	1.51E+07	1.75E+07	4.73E+07	3.00E+07	3.36E+07	7.42E+07	3.80E+07	3.34E+07
417	624.266571	2.514141098		3.73E+07	1.41E+07	1.82E+07	4990229.5	1.99E+07	4.63E+07	6.17E+07	3.82E+07	1467181.6	4664460.5	1.72E+07	5.23E+07	9505435	3.06E+07	1.45E+07	5.15E+07	3.19E+07
681	459.3106025	4.61080098	Ergokonin B	7696646.5	5097993.5	6487114	8023549	3.48E+07	1.70E+07	4.44E+07	7.00E+07	8308916.5	1.48E+07	7021781	1.62E+07	2.65E+07	2.22E+07	2.88E+07	7.72E+07	2.56E+07
673	654.3320887	4.659747059		1.51E+07	2.30E+07	1.45E+07	4873988.5	9729128	2.62E+07	2.93E+07	2.97E+07	4579606	6284409.5	2.17E+07	1.59E+07	1.70E+07	2.82E+07	2.12E+07	1.19E+08	2.70E+07
86	586.2298315	2.667653049		6.43E+07	3.63E+07	4.81E+07	4949733	8630320	4.21E+07	2.35E+07	1.05E+07	5143420.5	1.95E+07	2.82E+07	3.06E+07	1.32E+07	2.34E+07	9794069	5364017	2.27E+07
536	263.0550501	1.851977049	Cerdarin; 1-O-De-Me	1.89E+07	7785098	5009049.5	1.69E+08	2.40E+07	7822705	5561140.5	4491372	3.25E+08	1.20E+08	4273709.5	4718831	5558519	2.97E+07	6750982.5	1925433.3	3.03E+07
420	239.1641675	3.067175213	Eujavanoic acid B	6443053	1.08E+07	1.21E+07	1.08E+07	2.59E+07	1.42E+07	5.70E+07	1.00E+08	9694656	1.95E+07	1.15E+07	1.29E+07	2.01E+07	2.91E+07	1.88E+07	8.76E+07	2.72E+07

Molecular networks



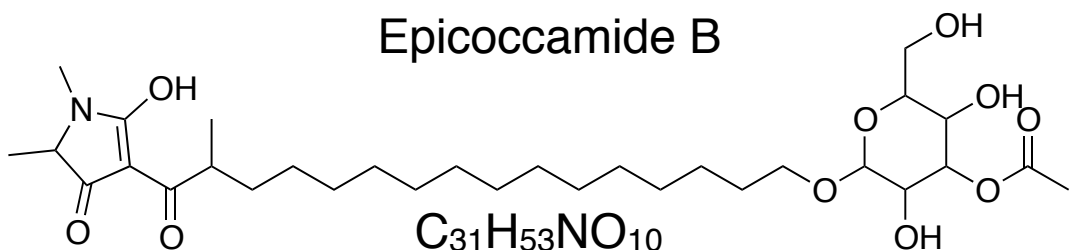


Epicoccum nigrum



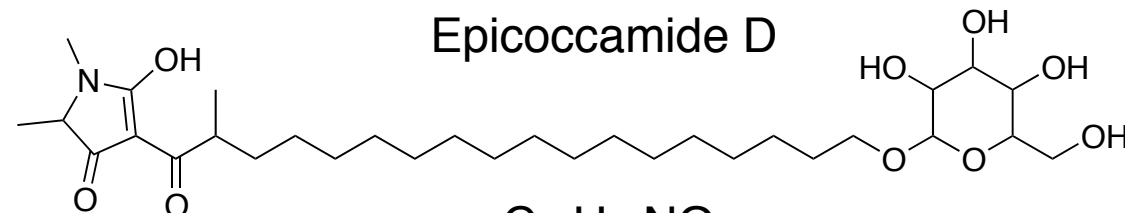
Epicoccum nigrum

Epicoccamide B



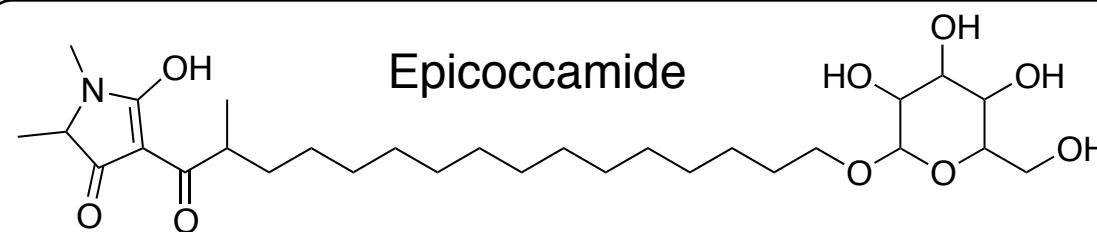
$C_{31}H_{53}NO_{10}$
599.37

Epicoccamide D

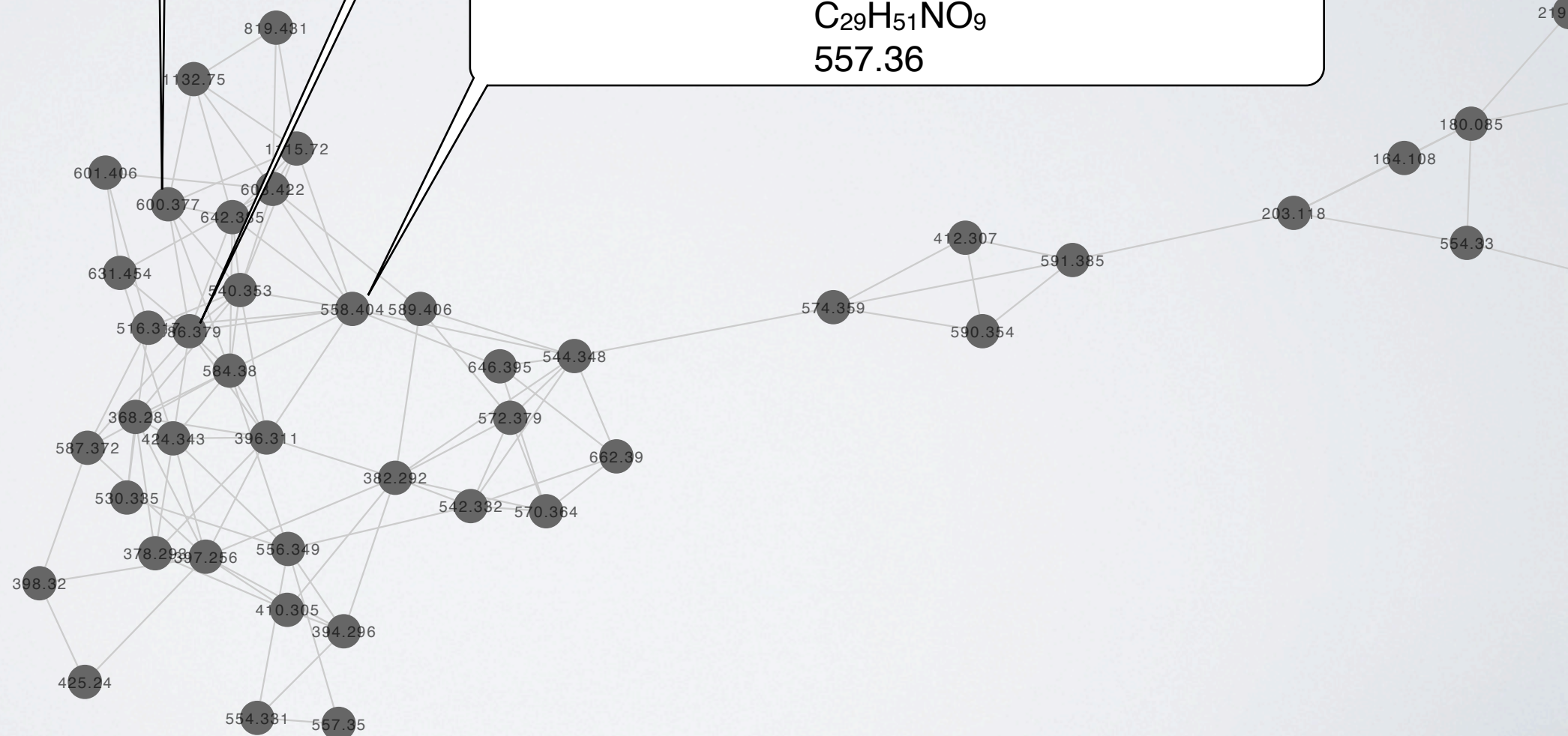


$C_{31}H_{55}NO_9$
585.39

Epicoccamide

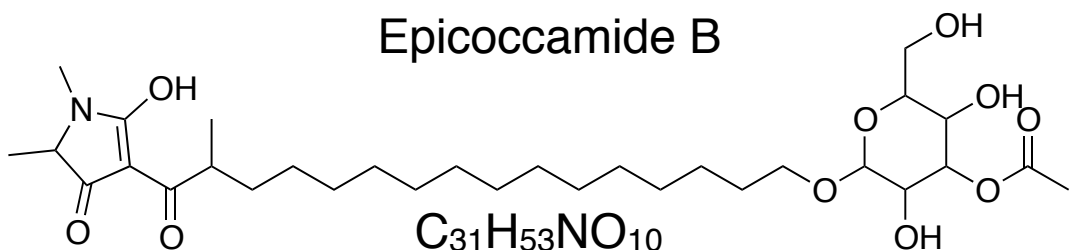


$C_{29}H_{51}NO_9$
557.36



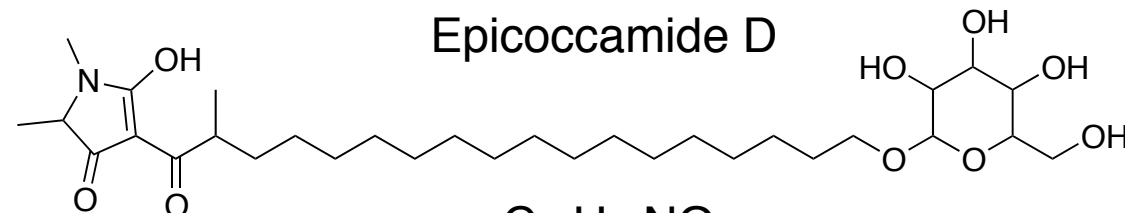
Epicoccum nigrum

Epicoccamide B



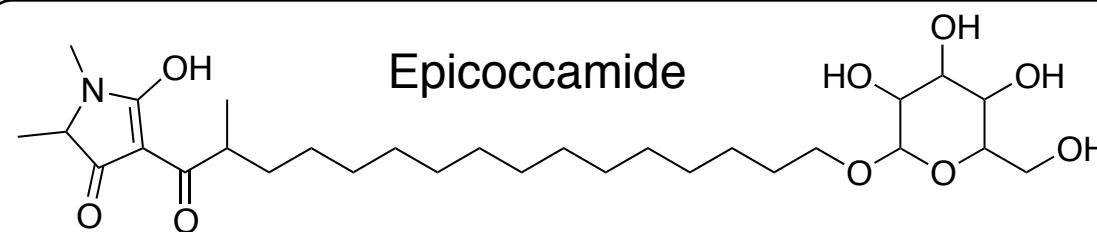
$C_{31}H_{53}NO_{10}$
599.37

Epicoccamide D

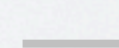
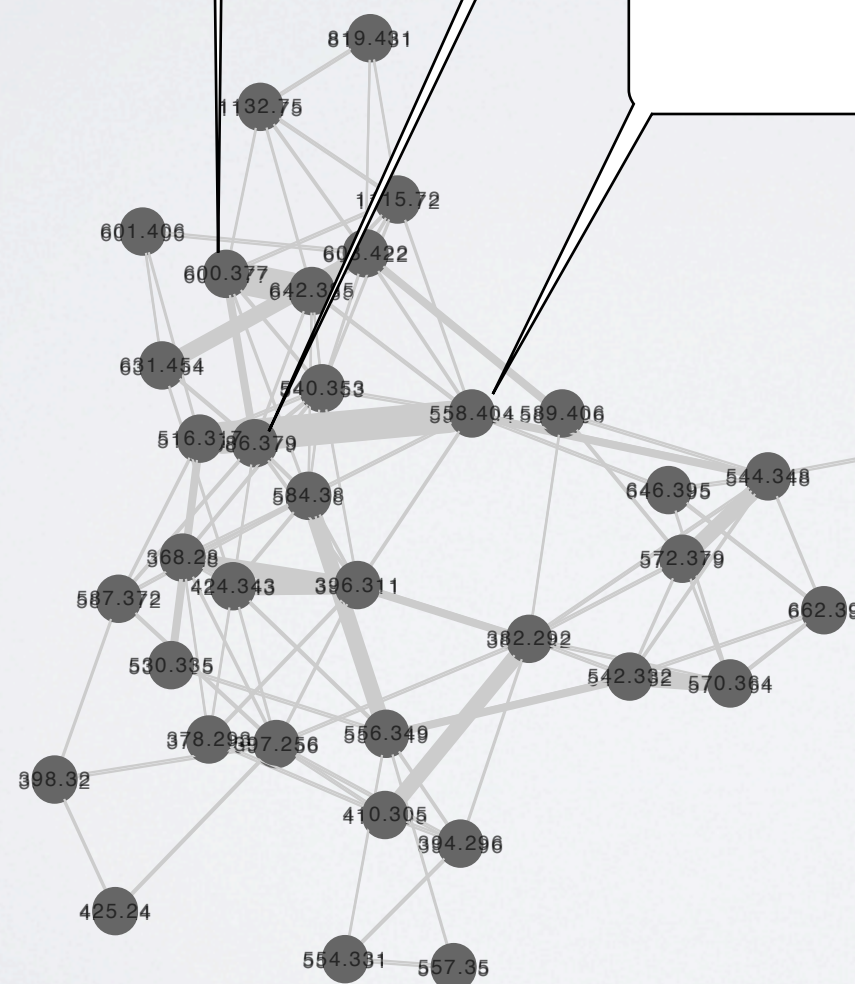


$C_{31}H_{55}NO_9$
585.39

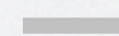
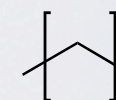
Epicoccamide



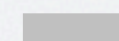
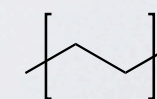
$C_{29}H_{51}NO_9$
557.36



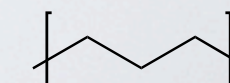
$\Delta m/z = 14$



$\Delta m/z = 28$



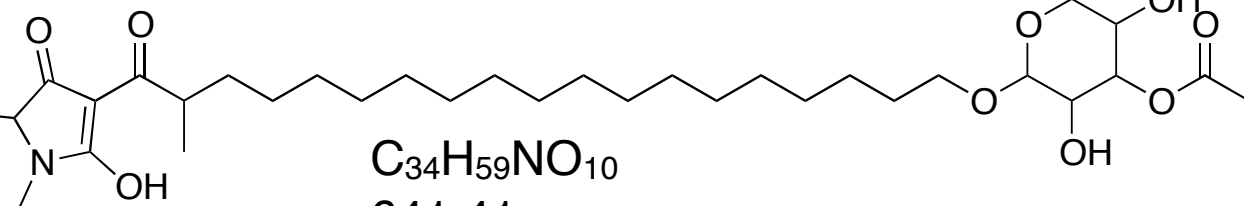
$\Delta m/z = 42$



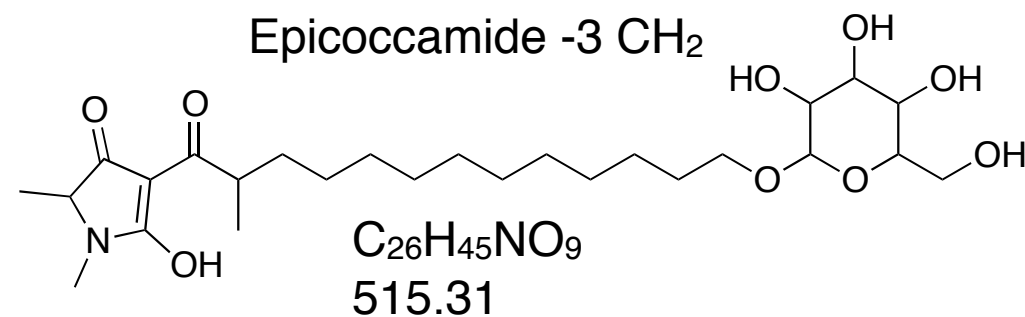
Epicoccum nigrum

Epicoccamide B

Epicoccamide B + 3CH₂

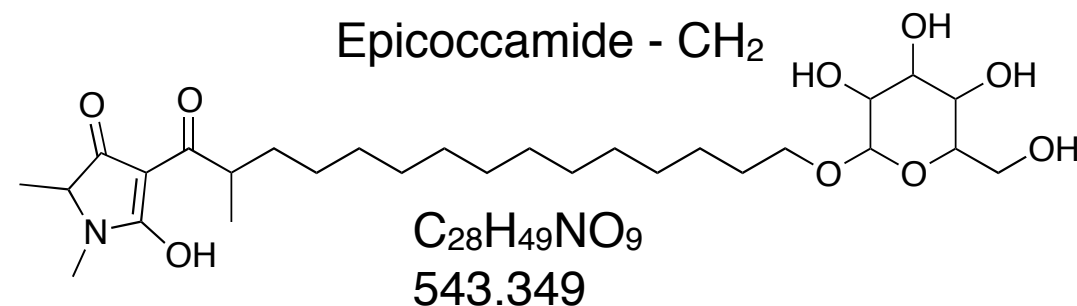


Epicoccamide -3 CH₂

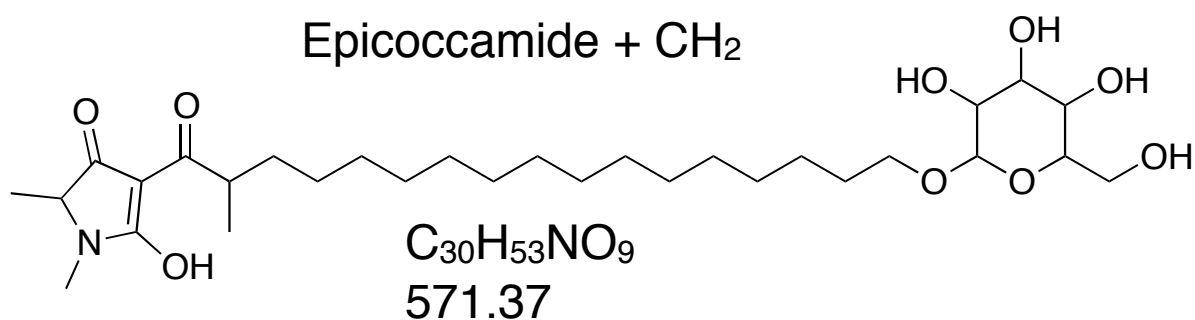


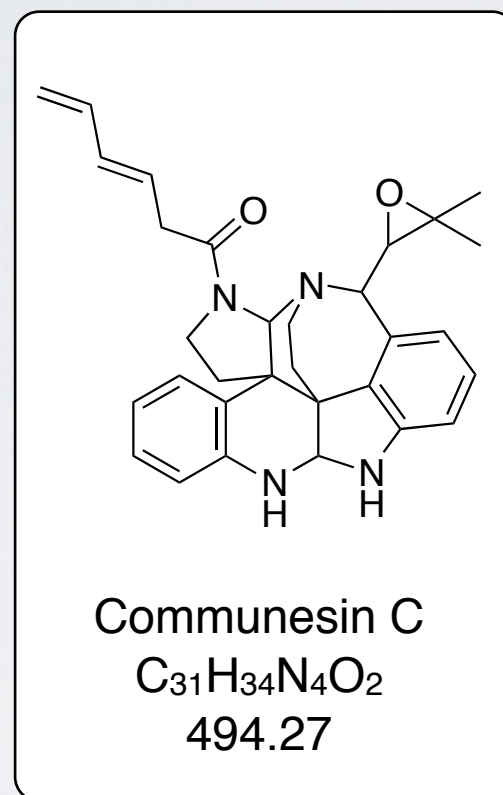
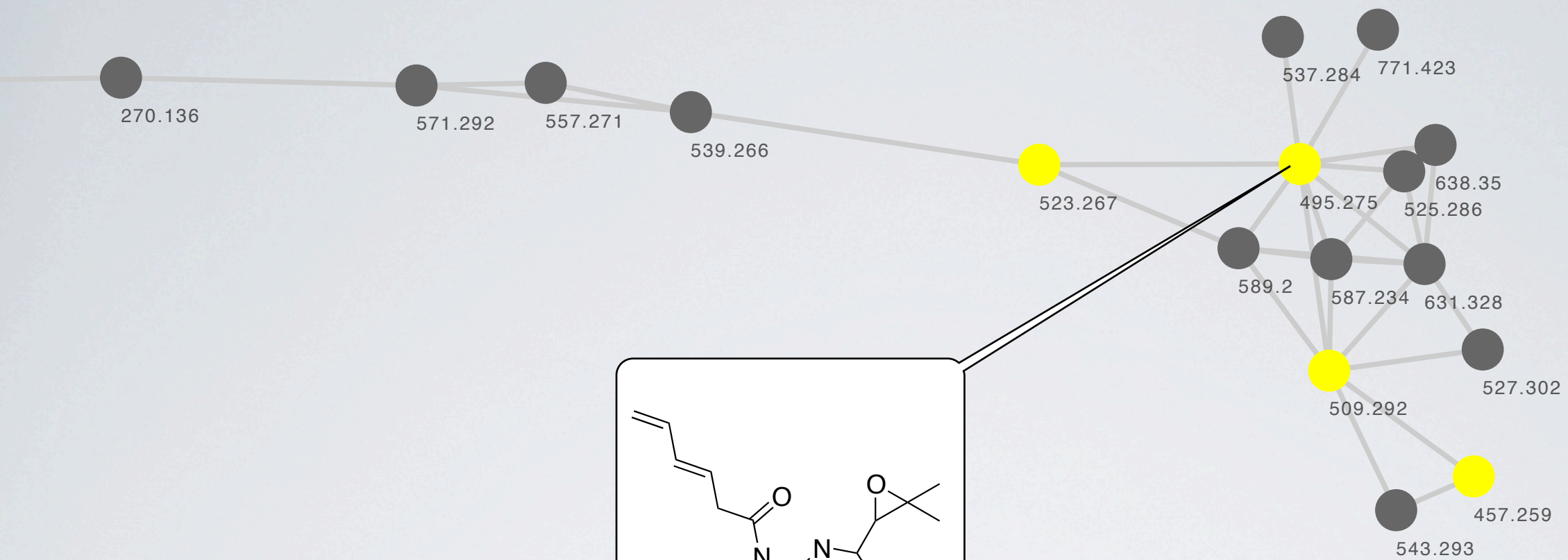
Epicoccamide

Epicoccamide - CH₂



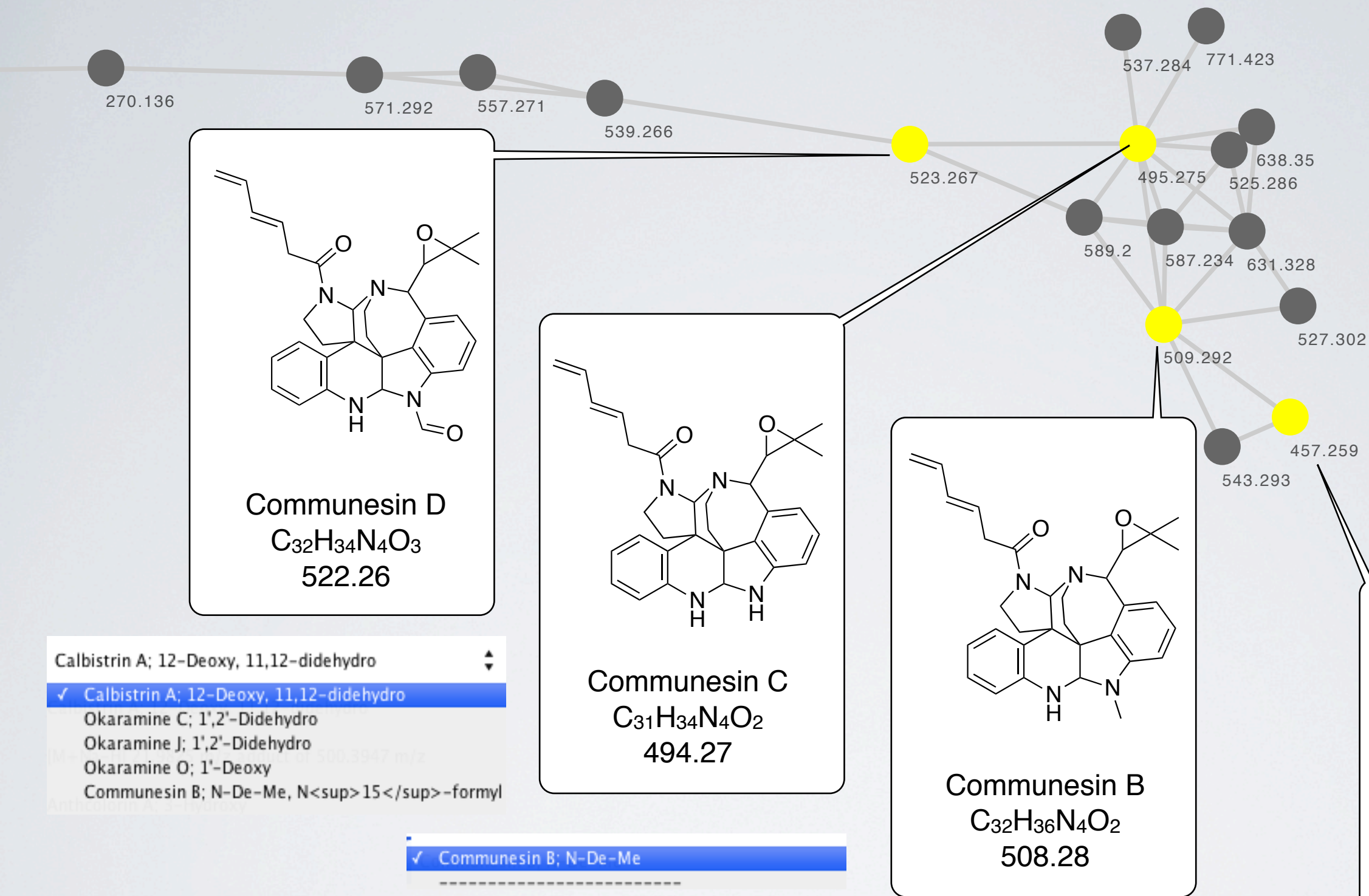
Epicoccamide + CH₂





✓ Communesin B; N-De-Me

Penicillium expansum



Xyloketal A

7-Hydroxy-25,26,27-trinor-3,
 Antibiotic F 2928-2
 Cohaerin F
 Cladobotric acid B; 12-Carbox
 Lucidenic acid N; 3,7-Diketone
 Communesin A
 7-Hydroxy-25,26,27-trinor-3,
 1-Hydroxy-8,12-dioxo-9,11(1

Calbistrin A; 12-Deoxy, 11,12-didehydro

✓ Calbistrin A; 12-Deoxy, 11,12-didehydro

Okaramine C; 1',2'-Didehydro

Okaramine J; 1',2'-Didehydro

Okaramine O; 1'-Deoxy

Communesin B; N-De-Me, N¹⁵-formyl

✓ Communesin B; N-De-Me

Amauromine

✓ Amauromine

Amauromine; Stereoisomer

Amauromine; 2,3-Diepimer

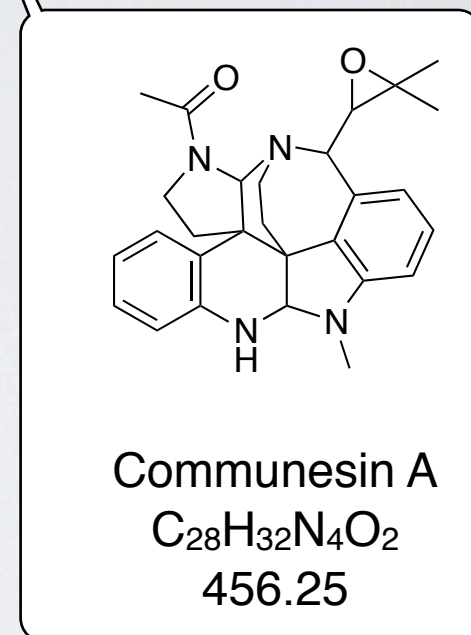
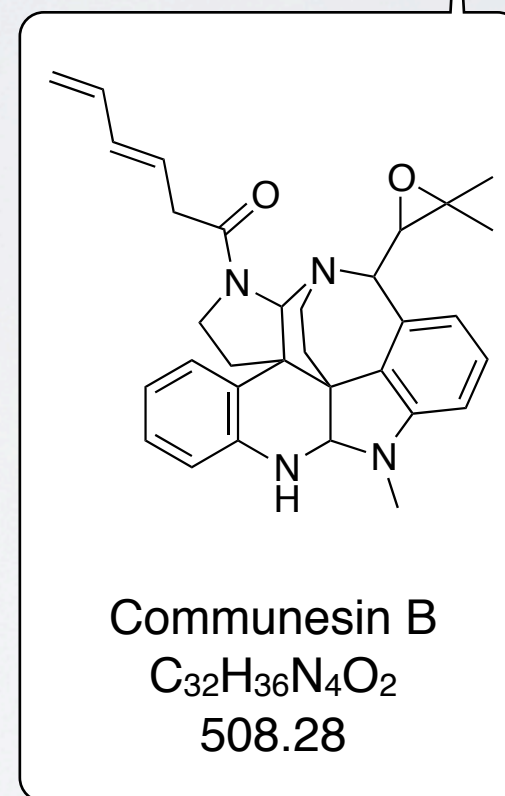
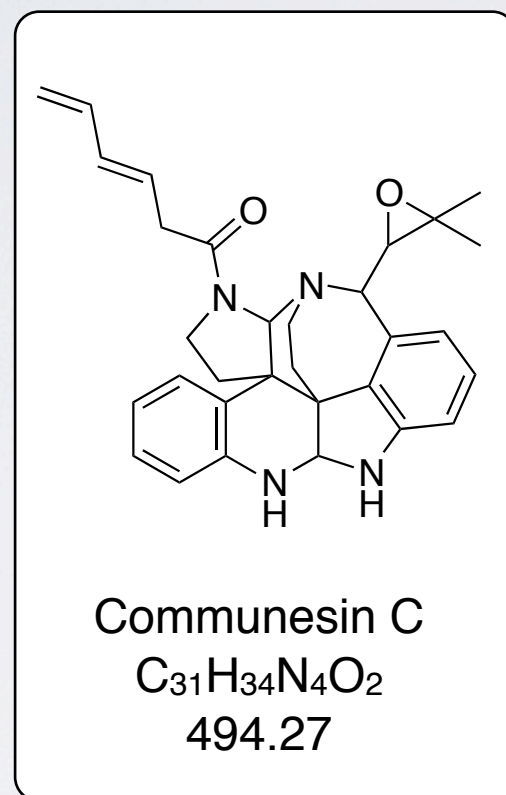
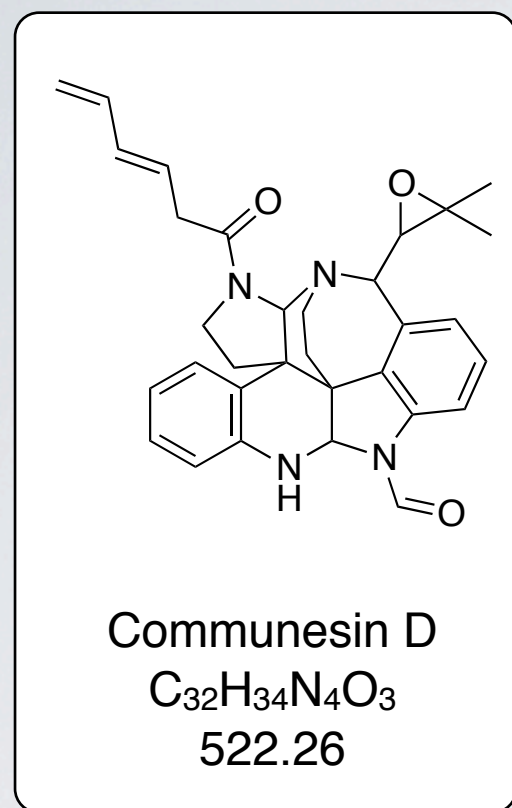
Communesin B

Fellutanine C

Fellutanine B; N¹-(1,1-Dimethyl-2-pr

Amauromine; 2,2',3,3'-Tetraepimer

Penicillium expansum



Xyloketal A

7-Hydroxy-25,26,27-trinor-3,
 Antibiotic F 2928-2
 Cohaerin F
 Cladobotric acid B; 12-Carbox
 Lucidenic acid N; 3,7-Diketone
 Communesin A
 7-Hydroxy-25,26,27-trinor-3,
 1-Hydroxy-8,12-dioxo-9,11(1

Calbistrin A; 12-Deoxy, 11,12-didehydro
 ✓ Calbistrin A; 12-Deoxy, 11,12-didehydro
 Okaramine C; 1',2'-Didehydro
 Okaramine J; 1',2'-Didehydro
 Okaramine O; 1'-Deoxy
 Communesin B; N-De-Me, N¹⁵-formyl

✓ Communesin B; N-De-Me

Amauromine
 ✓ Amauromine
 Amauromine; Stereoisomer
 Amauromine; 2,3-Diepimer
 Communesin B
 Fellutanine C
 Fellutanine B; N¹-(1,1-Dimethyl-2-pr
 Amauromine; 2,2',3,3'-Tetraepimer

Penicillium expansum

Penicillium vulpinum

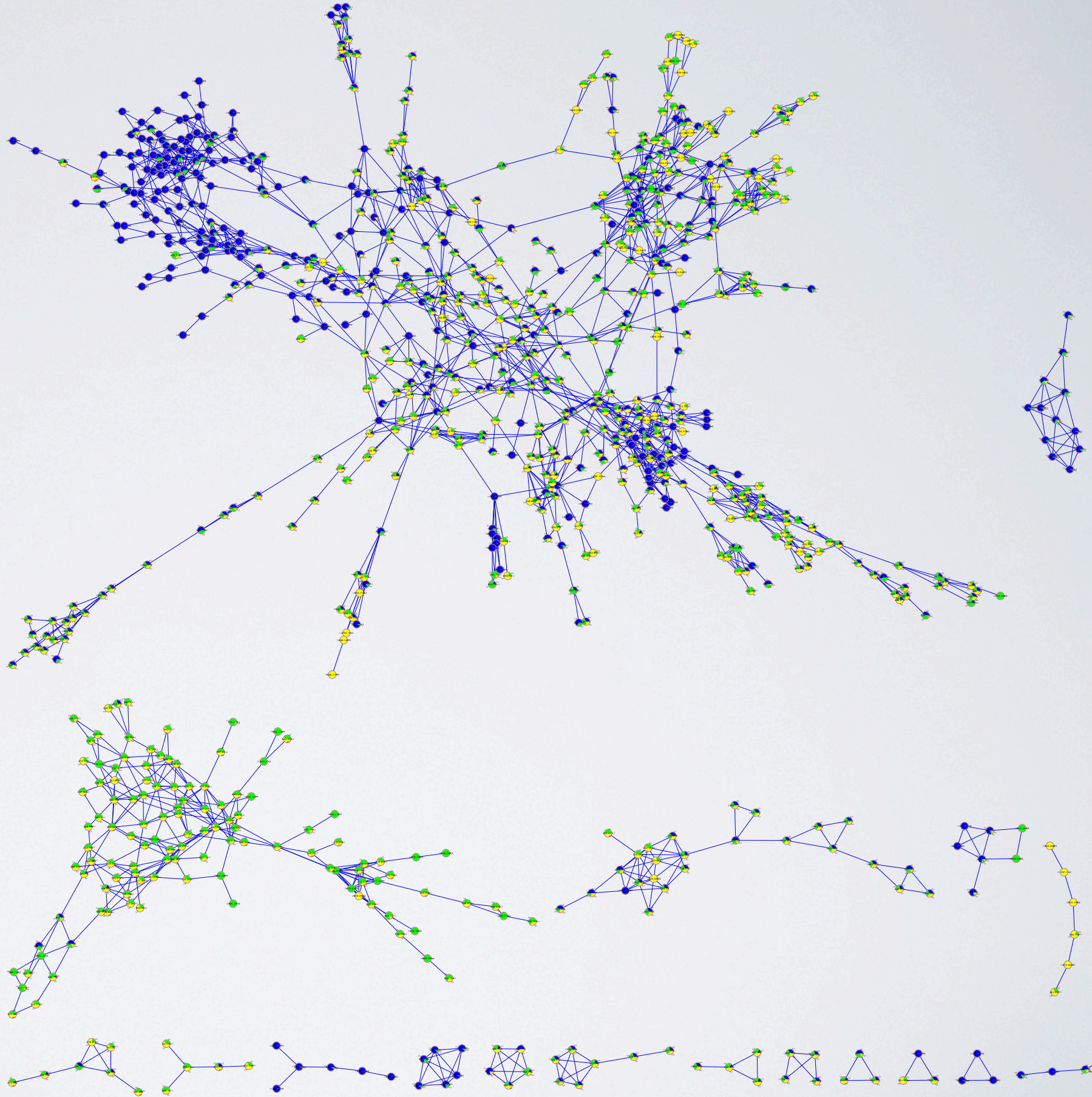
● 1st generation



● 2nd generation

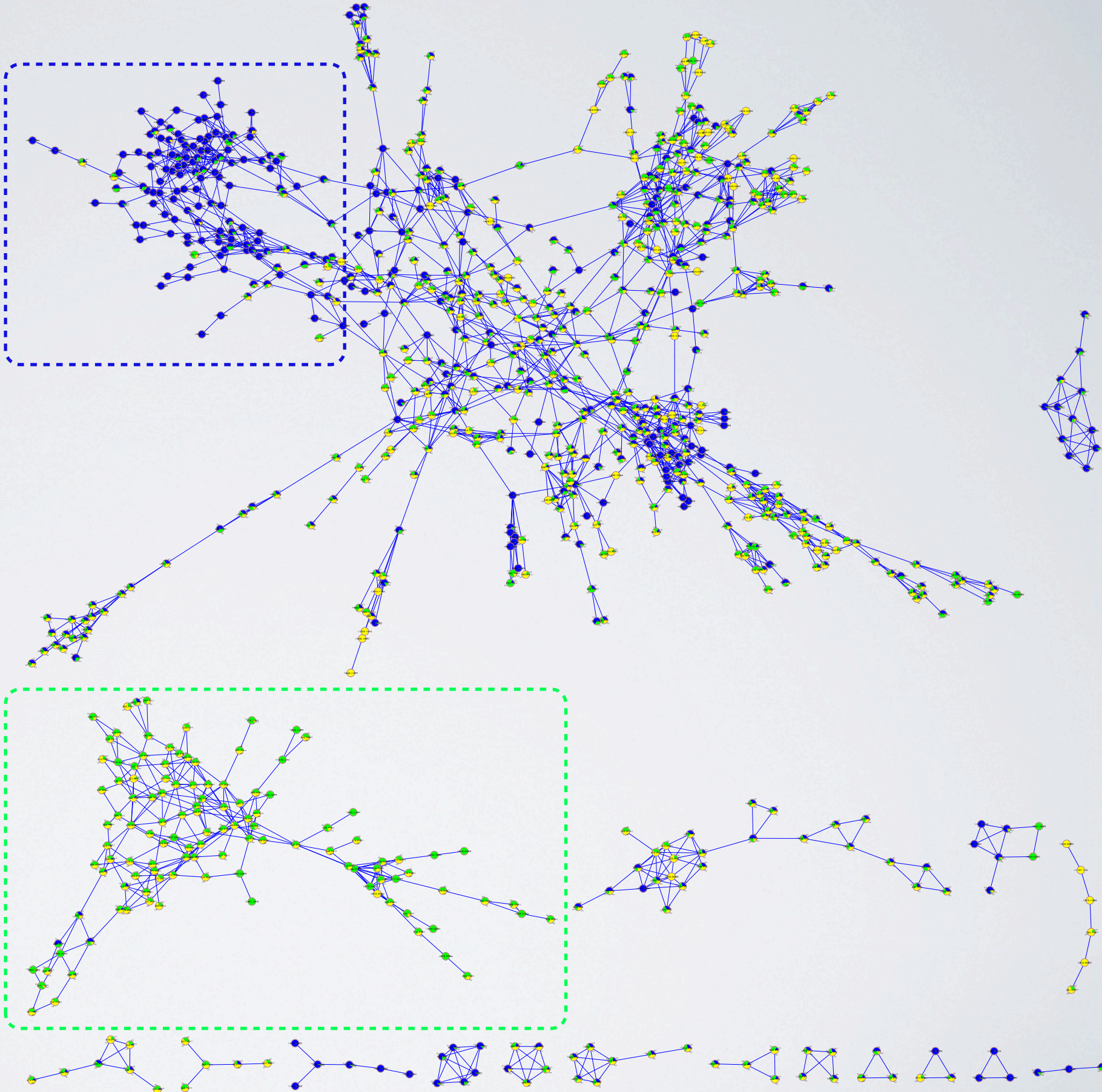


● 3rd generation



Penicillium vulpinum

- 1st generation
- 2nd generation
- 3rd generation

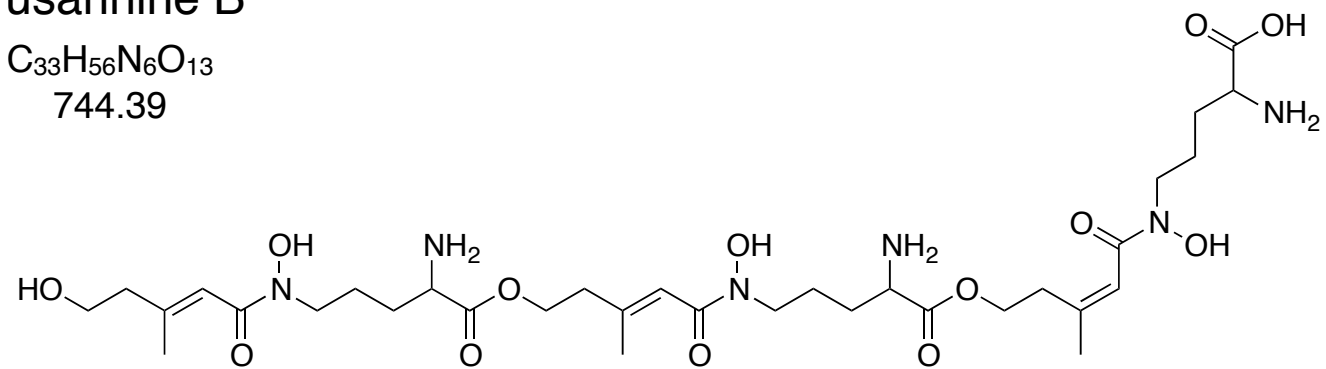


Penicillium vulpinum

Fusarinine B

$$\text{C}_{33}\text{H}_{56}\text{N}_6\text{O}_{13}$$

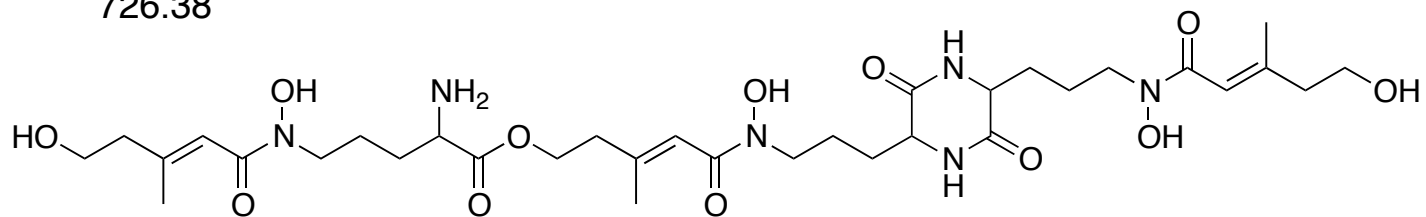
744.39



Coprogen B

$$\text{C}_{33}\text{H}_{54}\text{N}_6\text{O}_{12}$$

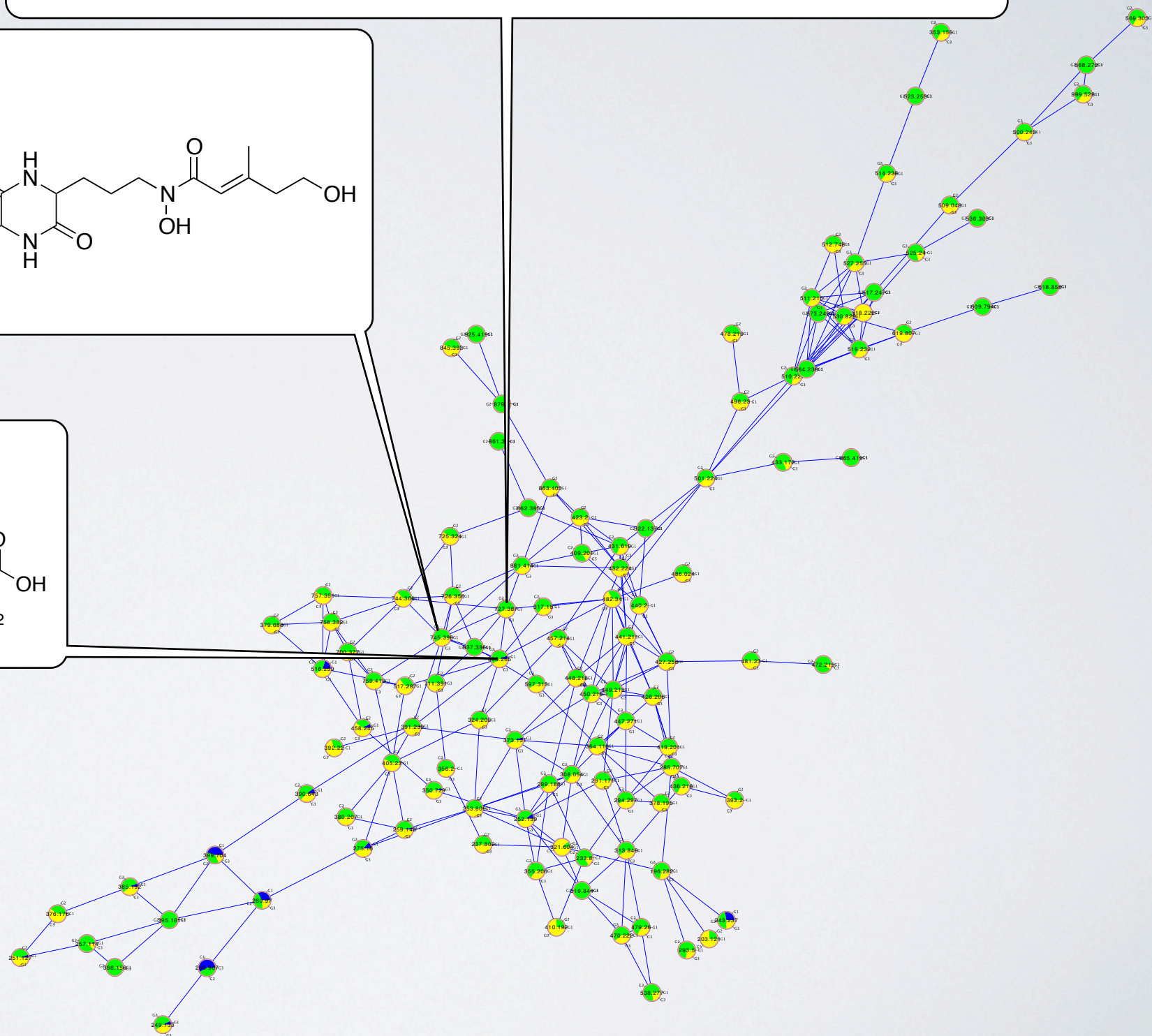
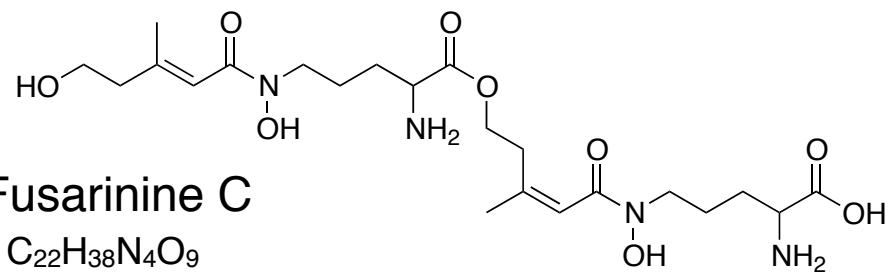
726.38



Fusarinine C

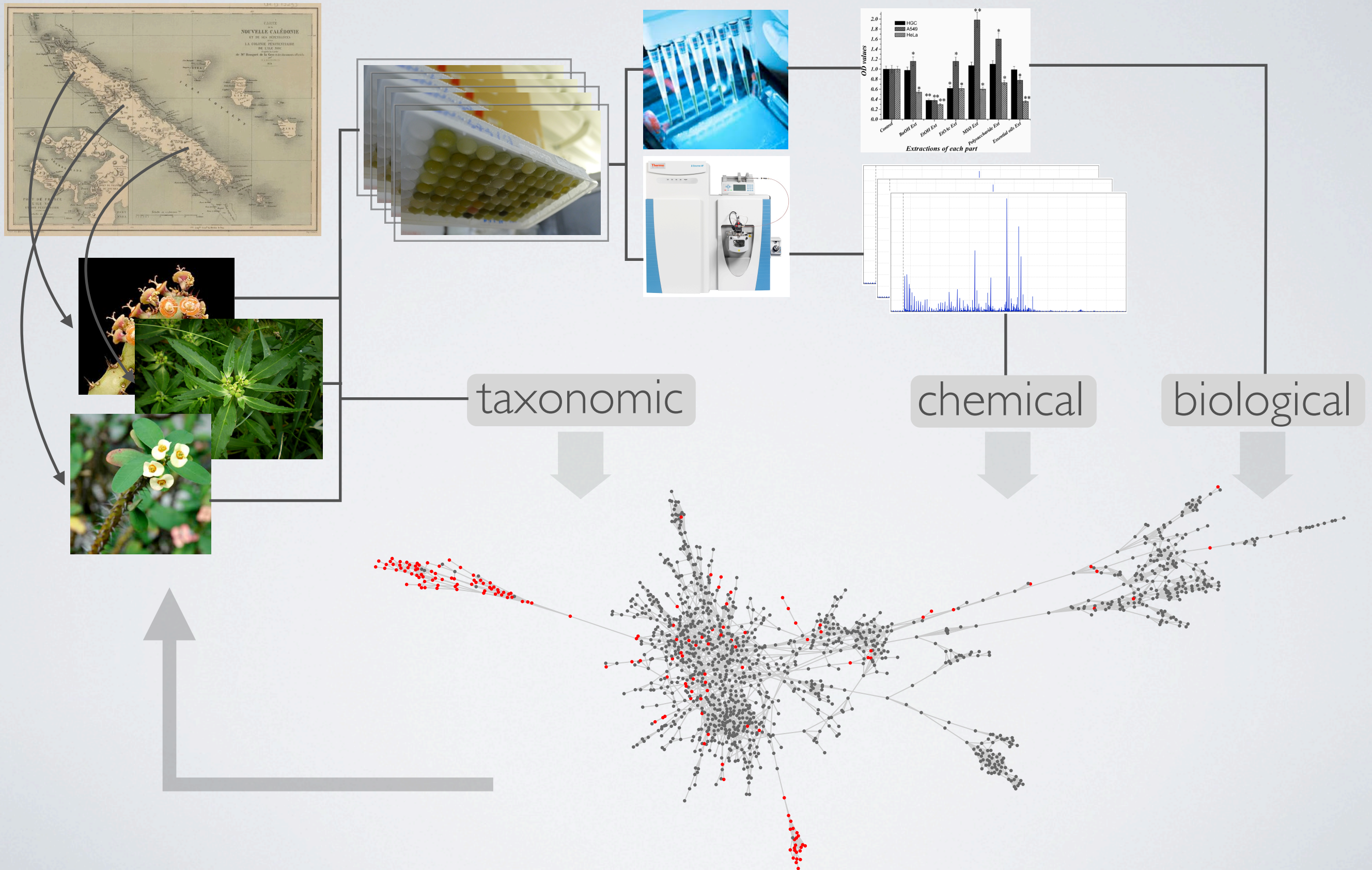
$$\text{C}_{22}\text{H}_{38}\text{N}_4\text{O}_9$$

502.26



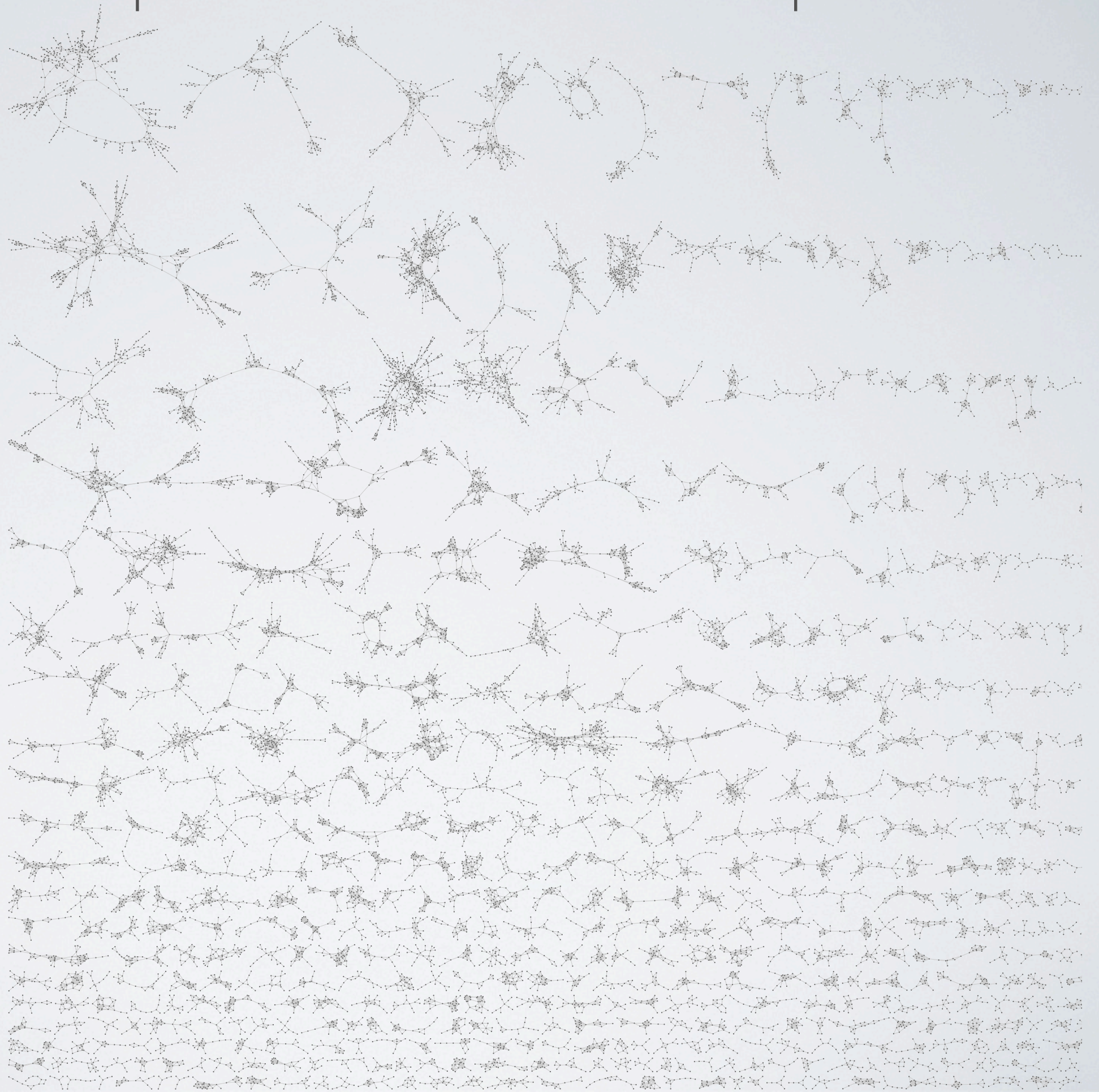
Neo-Caledonian Euphorbiaceae molecular maps

Collaborative project with Marc Litaudon and Louis-Félix Nothias (ICSN - Gif)



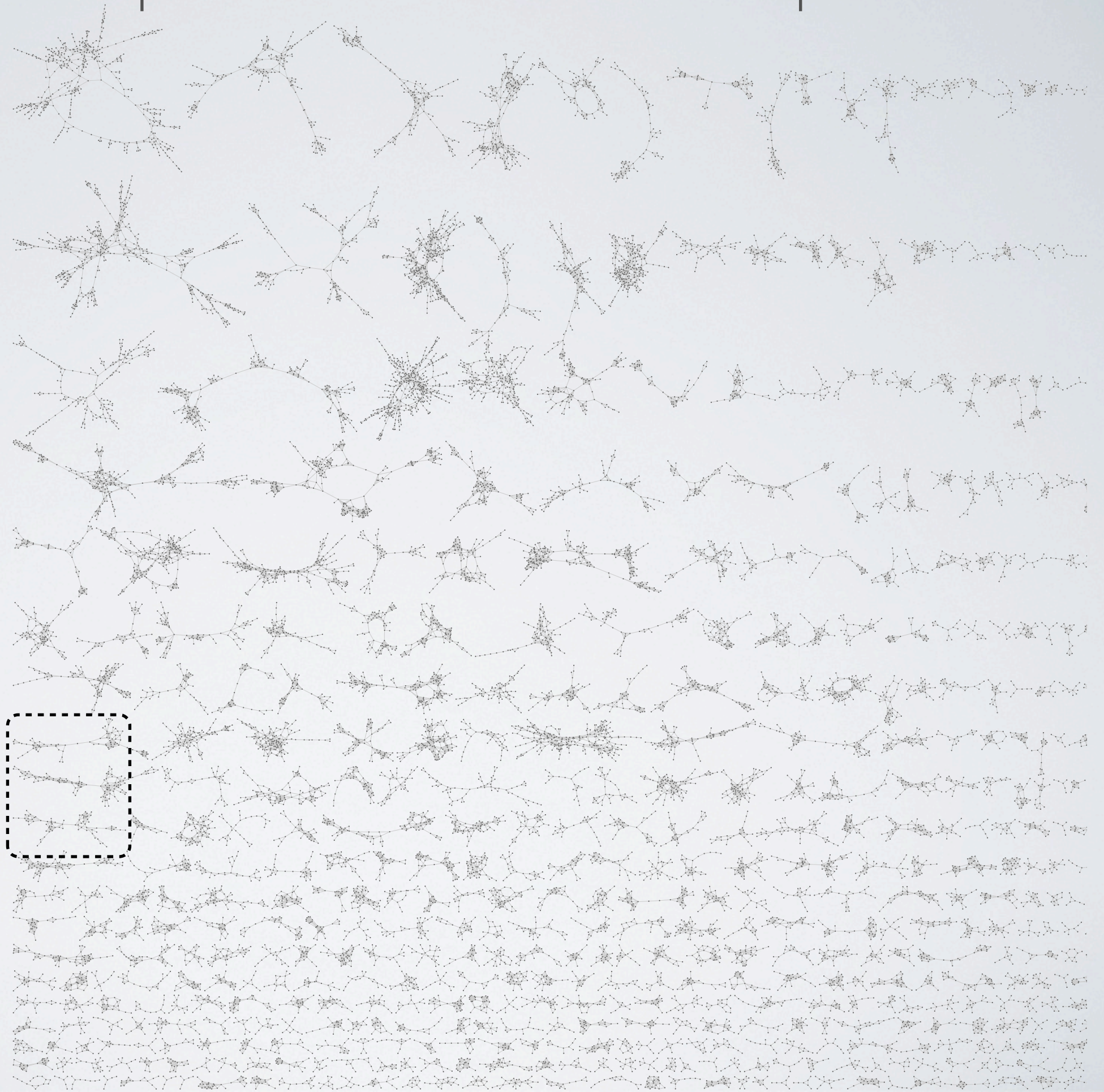
Neo-Caledonian Euphorbiaceae molecular maps

293 extracts
1.8 Mo MS²

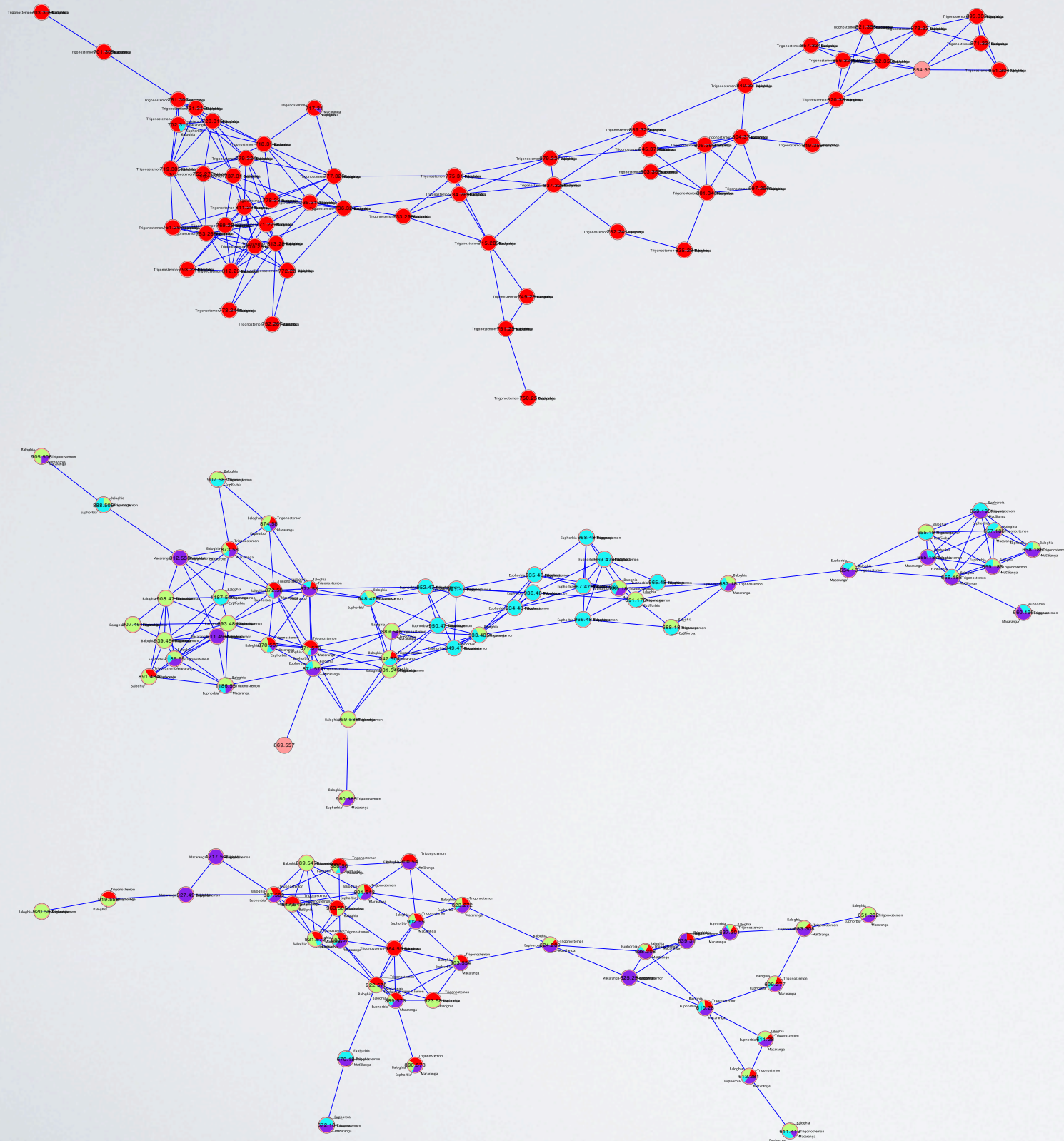


Neo-Caledonian Euphorbiaceae molecular maps

293 extracts
1.8 Mo MS²

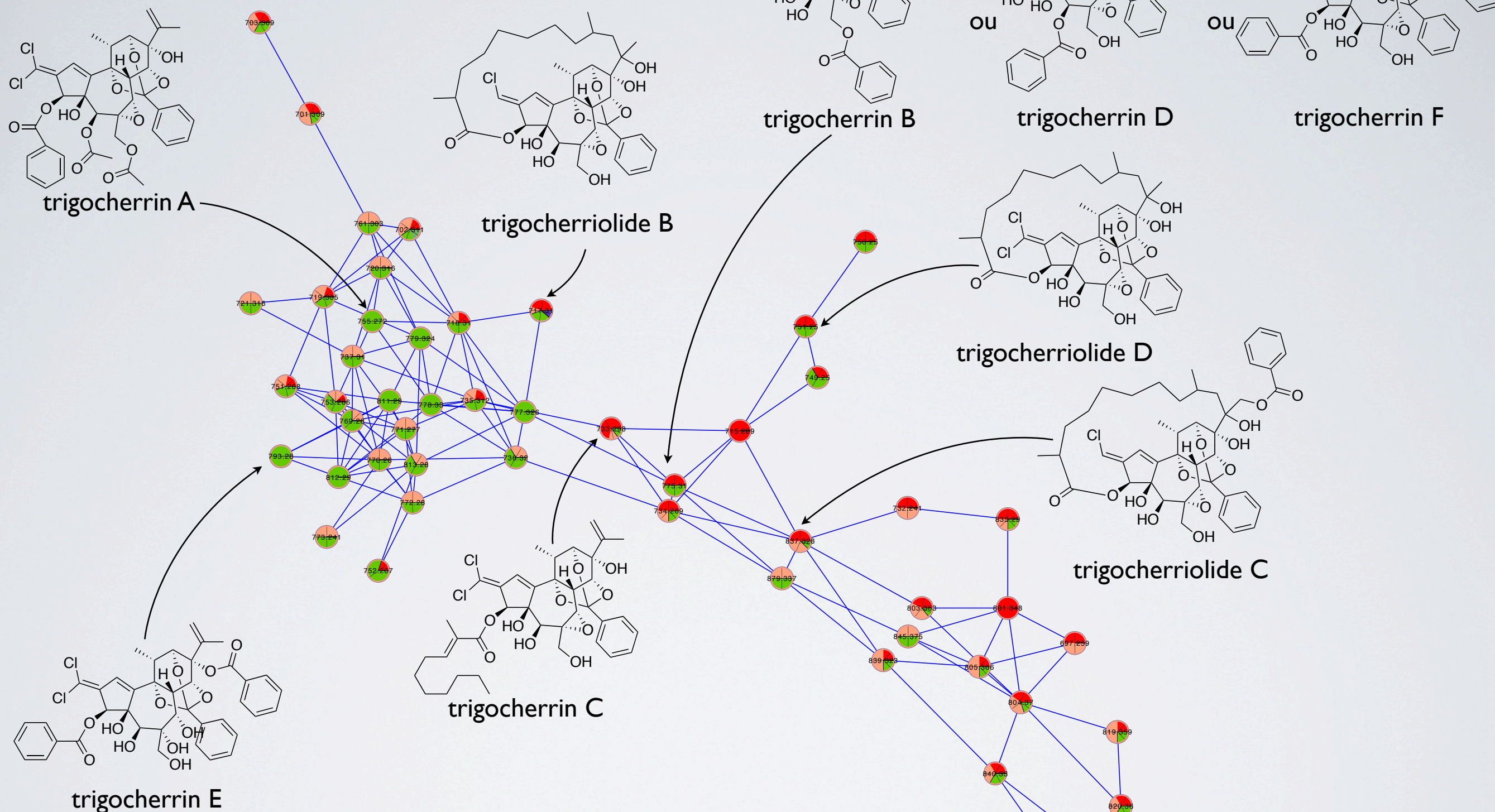


chemo-taxonomic input



- *Trigonostemon* sp.
- *Euphorbia* sp.
- *Baloghia* sp.
- *Macaranga* sp.

chemo-taxonomic input

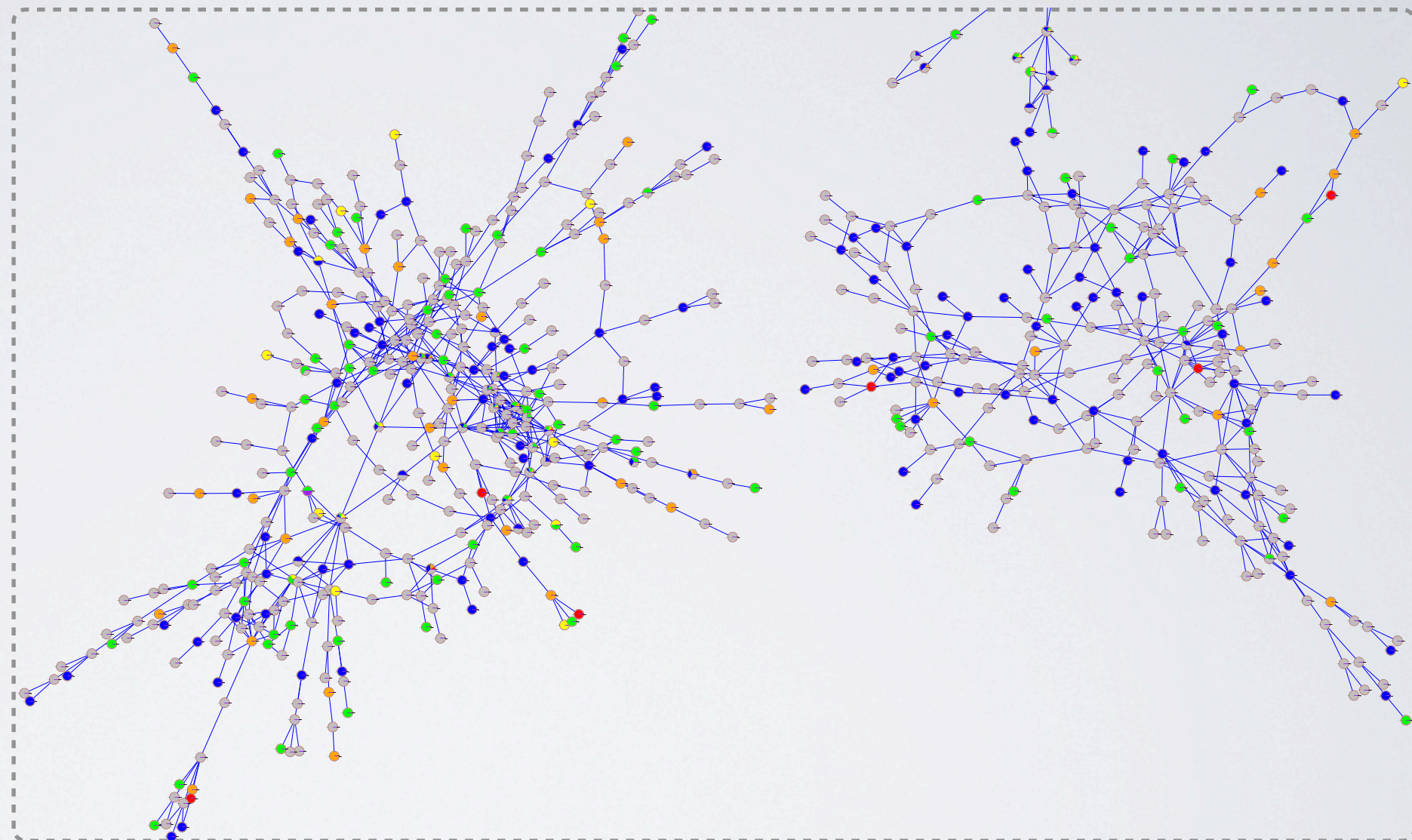


- *Trigonostemon cherrieri* (Bois)
- *Trigonostemon cherrieri* (Feuilles)
- *Trigonostemon cherrieri* (Ecorces)

This cluster is restricted to ions from *Trigonostemon cherrieri*. Various masses corresponding to trigocherrin and trigocherriolides series could be highlighted.

bio-chemical input

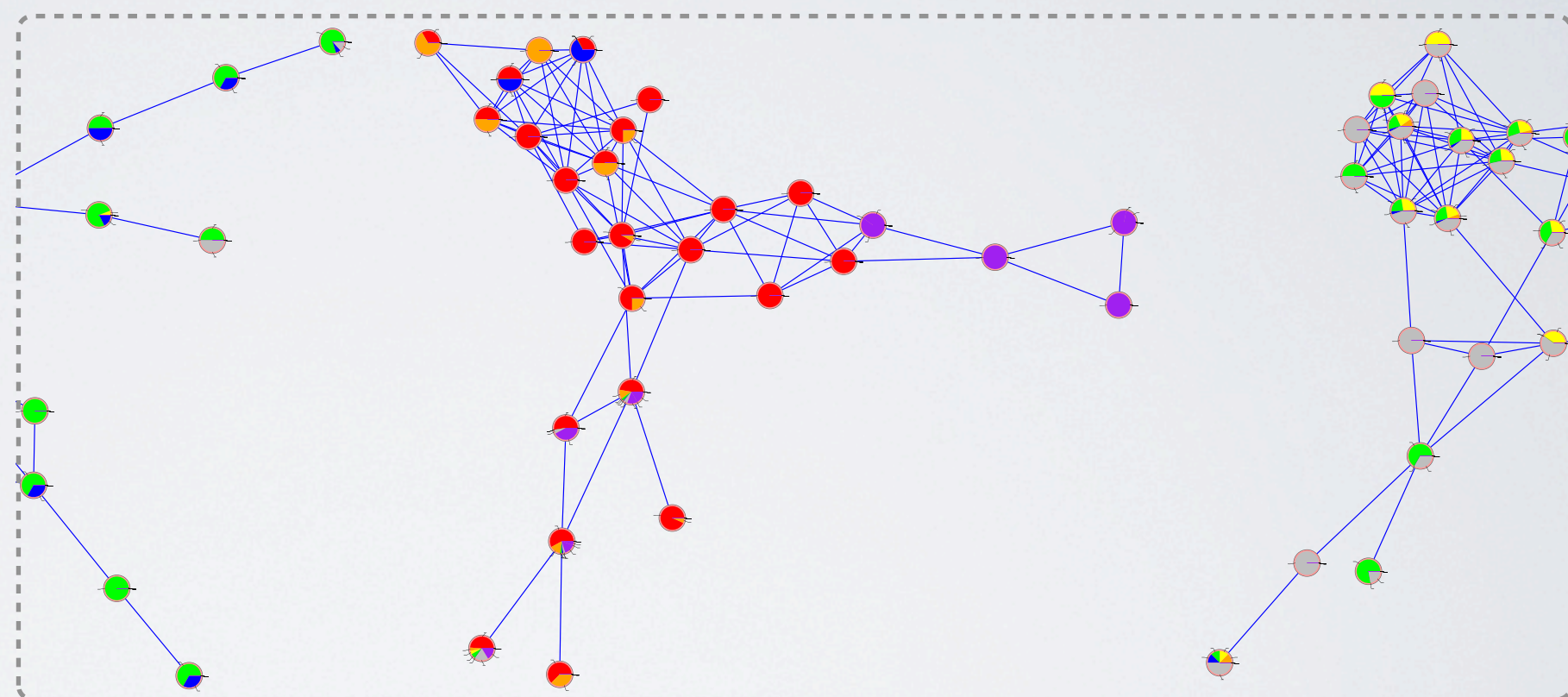
EC_{50} ($\mu\text{g/ml}$)



no specific pattern

bio-chemical input

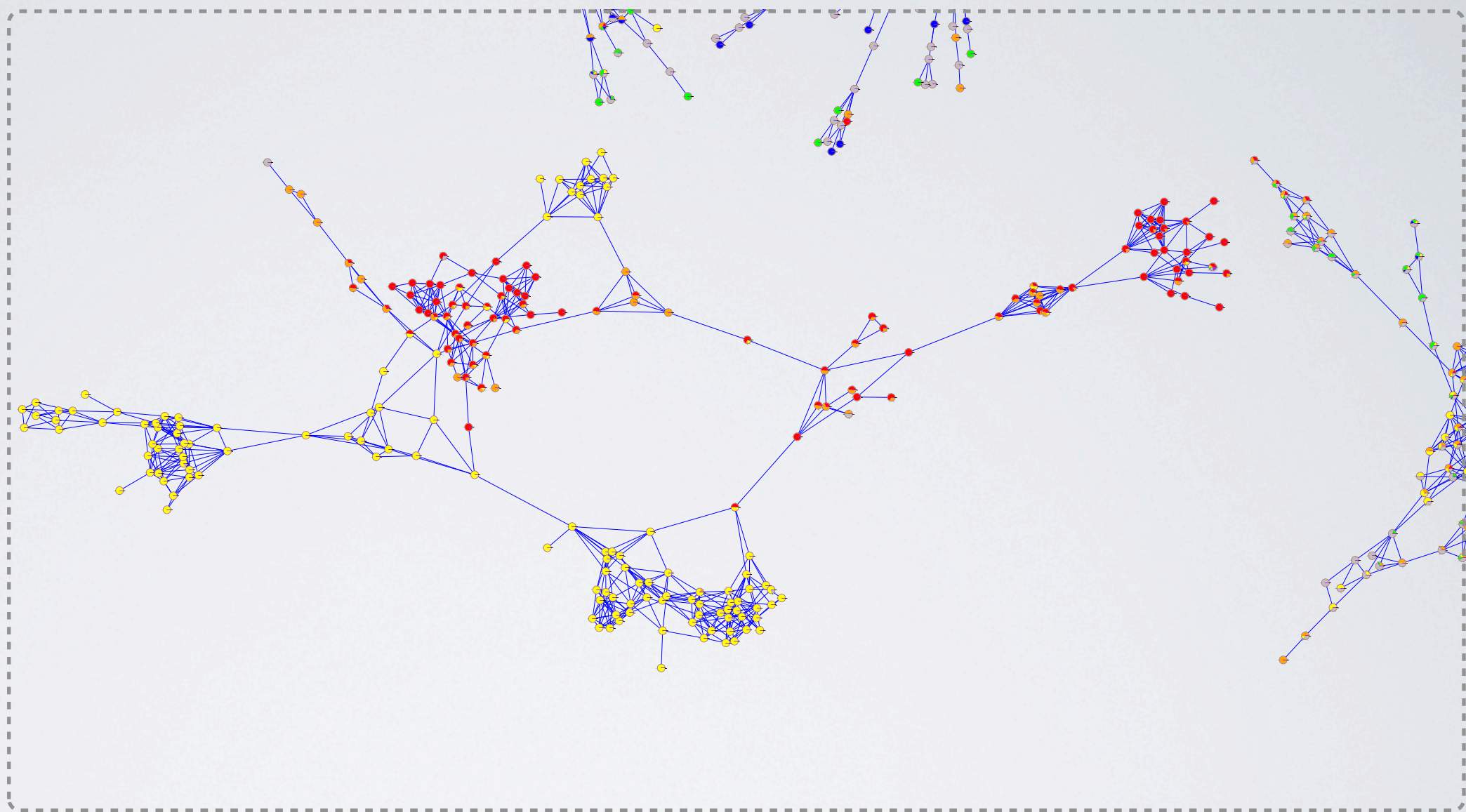
EC_{50} ($\mu\text{g/ml}$)



bioactive cluster matching standards

bio-chemical input

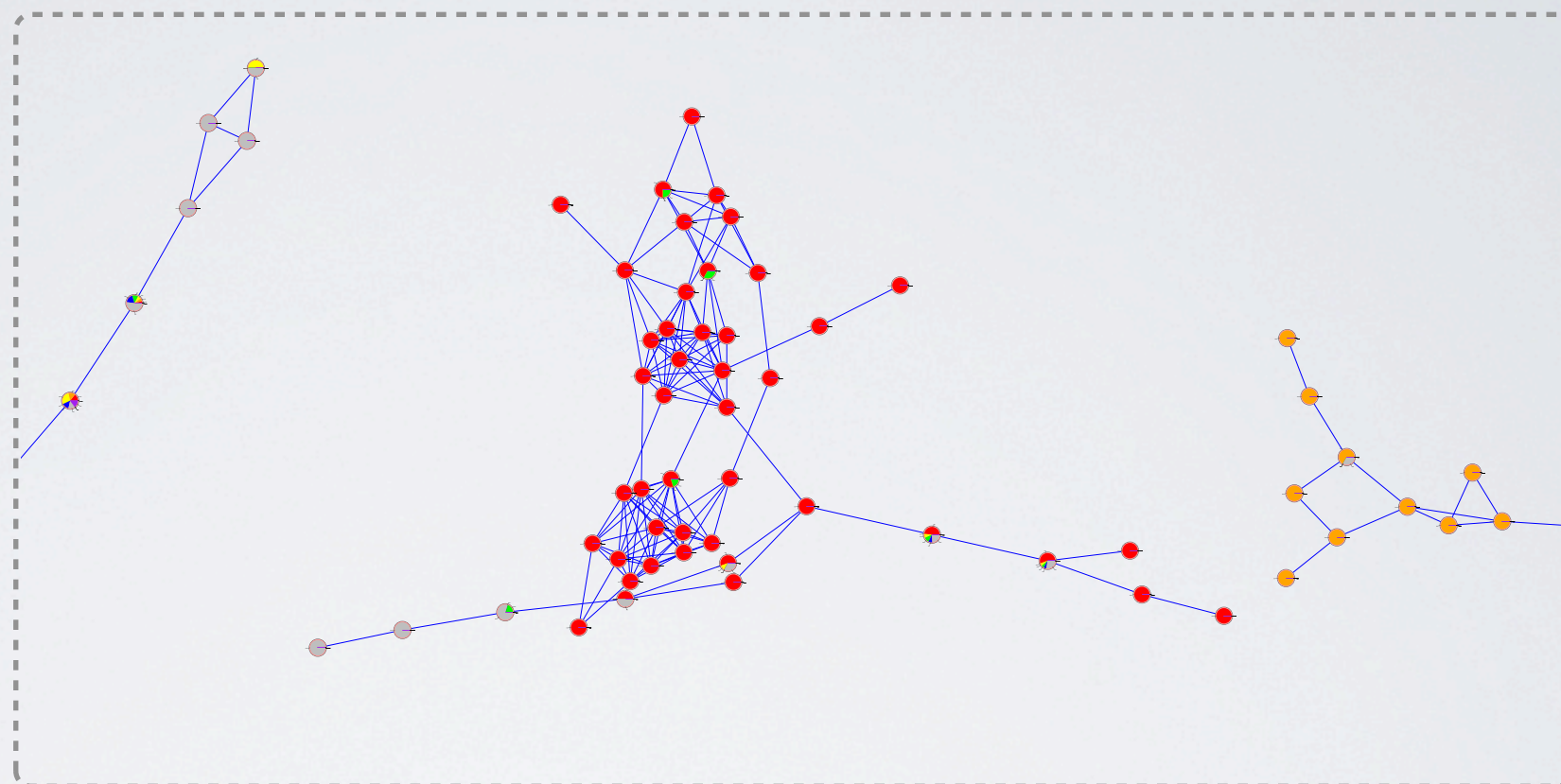
EC₅₀ (μg/ml)



bioactive cluster matching no standards

bio-chemical input

EC₅₀ (μg/ml)



bioactive cluster with unassayed analogues

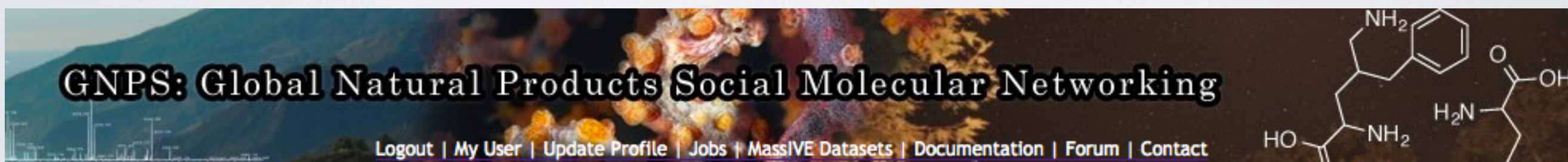
How to generate molecular networks

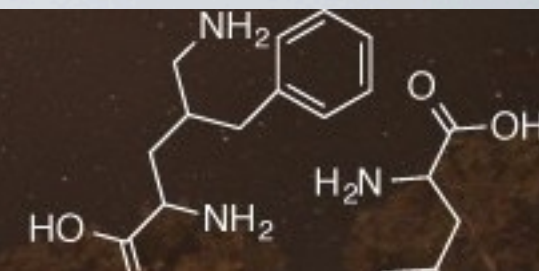
On your laptop :

Spectral Networks package - UCSD Bioinformatics

<http://usa.ucsd.edu:8080/projects/sps/jcanhita/Download/sps.html>

Online : GNPS <http://gnps.ucsd.edu>

A banner image for GNPS (Global Natural Products Social Molecular Networking). The background features a colorful, abstract molecular structure. On the left, there is a small inset showing a mass spectrum plot. The text "GNPS: Global Natural Products Social Molecular Networking" is prominently displayed in the center. Below this, a navigation bar includes links: "Logout | My User | Update Profile | Jobs | Massive Datasets | Documentation | Forum | Contact". On the right side of the banner, there is a chemical structure of a complex molecule, possibly a peptide or a natural product derivative, with various functional groups like amino groups and carboxylic acid groups labeled.



Continuous dereplication process

MassIVE Dataset MSV000079034 GNPS_New_Caledonian_Euphorbiaceae_part1

Reporting 0.9309542% more IDs and 12 more IDs

0.0% different IDs and 0 different IDs

0.0% deleted IDs and 0 deleted IDs

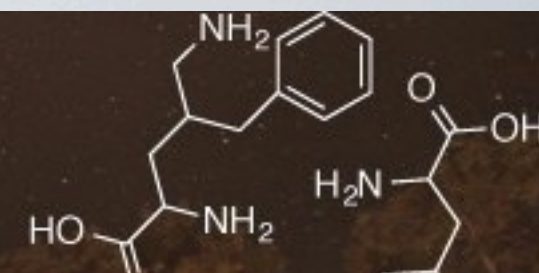
with 1289 total

Results are available at:

<http://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=2e0415c4ad5846c9b15198de7491ad77>

The dataset is available at:

http://gnps.ucsd.edu/ProteoSAFe/result.jsp?task=3b3a30dd21bb48f8a05b10e855b317c7&view=group_all_annotations



Continuous dereplication process

Job Status

Workflow MOLECULAR-CONTINUOUS-ID

Status DONE
[Clone]
[]

Identifications

[[Different Identifications](#) | [New Identifications](#) | [Deleted Identifications](#) | [All Identifications](#)]

Network Views

[[Explore Network](#) | [Explore Network Pairs](#)]

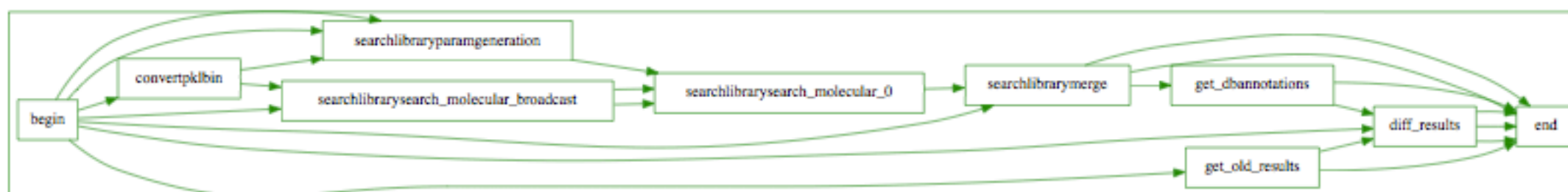
User continuous (mwang87@gmail.com), continuous

Title Continuous ID Search: MSV000079034

Date Created 2015-04-30 10:56:30.0

Execution Time 12 minutes 57 seconds

Progress



Continuous dereplication process

 8	ViewLib		★ ★ ★ ☆	14391	1	0.74348	m/z 295 of diterpene esters (collected from 12-deoxyphorbol-13-acetate)	Litaudon-Wolfender	Nothias-Allard	Bronze	10	934.03	0.276	295.169	
 9	ViewLib		★ ★ ★ ☆	21363	1	0.73186	m/z 313 of diterpene esters (collected from 12-deoxyphorbol-13-acetate)	Litaudon-Wolfender	Nothias-Allard	Bronze	9	1320.57	0.414	313.179	
 10	ViewLib		★ ★ ★ ☆	21291	1	0.71676	m/z 313 of diterpene esters (collected from 12-deoxyphorbol-13-acetate)	Litaudon-Wolfender	Nothias-Allard	Bronze	9	106.70	0.033	313.179	
 11	ViewLib		☆ ☆ ☆ ☆	90879	1	0.70968	Pheophytin	Pieter C. Dorrestein	Don D. Nguyen	Bronze	7	21.85	0.019	871.593	
 12	ViewLib		★ ★ ★ ☆	14384	1	0.70702	m/z 295 of diterpene esters (collected from 12-deoxyphorbol-13-acetate)	Litaudon-Wolfender	Nothias-Allard	Bronze	9	1398.14	0.413	295.169	

Merci pour votre attention !