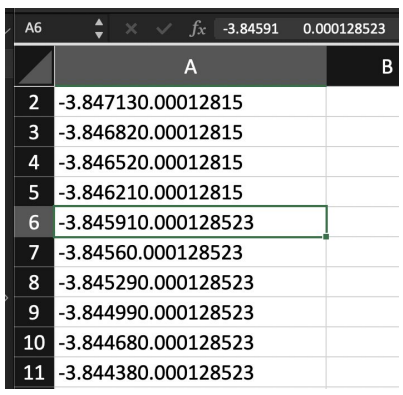
MestreNova

TopSpin

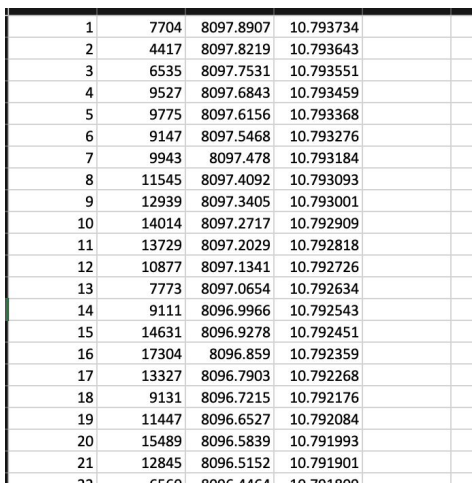
Spectra Files

Tab-delimited CSV file
Two columns: ppm shift and intensity

CSV file
Many columns



	A	B
2	-3.847130.00012815	
3	-3.846820.00012815	
4	-3.846520.00012815	
5	-3.846210.00012815	
6	-3.845910.000128523	
7	-3.84560.000128523	
8	-3.845290.000128523	
9	-3.844990.000128523	
10	-3.844680.000128523	
11	-3.844380.000128523	



1	7704	8097.8907	10.793734	
2	4417	8097.8219	10.793643	
3	6535	8097.7531	10.793551	
4	9527	8097.6843	10.793459	
5	9775	8097.6156	10.793368	
6	9147	8097.5468	10.793276	
7	9943	8097.478	10.793184	
8	11545	8097.4092	10.793093	
9	12939	8097.3405	10.793001	
10	14014	8097.2717	10.792909	
11	13729	8097.2029	10.792818	
12	10877	8097.1341	10.792726	
13	7773	8097.0654	10.792634	
14	9111	8096.9966	10.792543	
15	14631	8096.9278	10.792451	
16	17304	8096.859	10.792359	
17	13327	8096.7903	10.792268	
18	9131	8096.7215	10.792176	
19	11447	8096.6527	10.792084	
20	15489	8096.5839	10.791993	
21	12845	8096.5152	10.791901	

`import_nmr_spectra_data()`
Import and combine spectra files
Clean and make x,y matrix of ppm and intensity

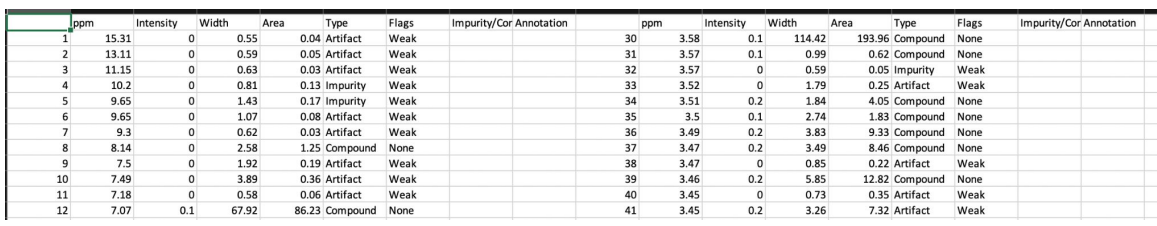
`assign_compound_classes_v2()`
Assign chemical classes/bins to each peak

`gg_spectra()`
Make simple graphs

`compute_relabund_cores(method = "AUC")`
Calculate relative abundance from spectra, integrating AUC for each region

Peaks Files

MNova, v1: Peaks info spread across multiple column-groups
`process_peaks(method = "multiple columns")`

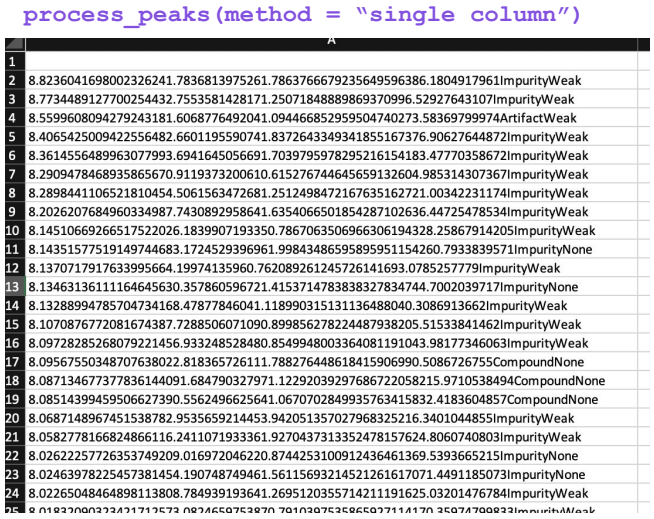


	ppm	Intensity	Width	Area	Type	Flags	Impurity/Cor	Annotation		ppm	Intensity	Width	Area	Type	Flags	Impurity/Cor	Annotation
1	15.31	0	0.55	0.04	Artifact	Weak			30	3.58	0.1	114.42	193.96	Compound	None		
2	13.11	0	0.59	0.05	Artifact	Weak			31	3.57	0.1	0.99	0.62	Compound	None		
3	11.15	0	0.63	0.03	Artifact	Weak			32	3.57	0	0.59	0.05	Impurity	Weak		
4	10.2	0	0.81	0.13	Impurity	Weak			33	3.52	0	1.79	0.25	Artifact	Weak		
5	9.65	0	1.43	0.17	Impurity	Weak			34	3.51	0.2	1.84	4.05	Compound	None		
6	9.65	0	1.07	0.08	Artifact	Weak			35	3.5	0.1	2.74	1.83	Compound	None		
7	9.3	0	0.62	0.03	Artifact	Weak			36	3.49	0.2	3.83	9.33	Compound	None		
8	8.14	0	2.58	1.25	Compound	None			37	3.47	0.2	3.49	8.46	Compound	None		
9	7.5	0	1.92	0.19	Artifact	Weak			38	3.47	0	0.85	0.22	Artifact	Weak		
10	7.49	0	3.89	0.36	Artifact	Weak			39	3.46	0.2	5.85	12.82	Compound	None		
11	7.18	0	0.58	0.06	Artifact	Weak			40	3.45	0	0.73	0.35	Artifact	Weak		
12	7.07	0.1	67.92	86.23	Compound	None			41	3.45	0.2	3.26	7.32	Artifact	Weak		

`process_peaks()`
Import and combine peaks files. Clean.

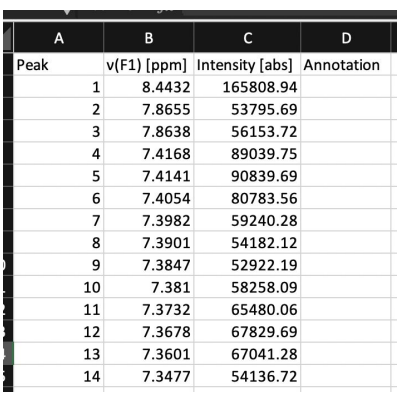
`assign_compound_classes_v2()`
Assign chemical classes/bins to each peak

MNova, v2: Tab-delim, peaks info in single column, no column headers
`process_peaks(method = "single column")`



	A
1	
2	8.8236041698002326241.7836813975261.7863766679235649596386.1804917961ImpurityWeak
3	8.7734489127700254432.7553581428171.2507184888986937096.52927643107ImpurityWeak
4	8.5599608094279243181.6068776492041.0944668529595047402 73.58369799974ArtifactWeak
5	8.4065425009422556482.6601195590741.8372643349341855167376.90627644872ImpurityWeak
6	8.3614556489963077993.6941645056691.7039795978295216154183.47770358672ImpurityWeak
7	8.2909478468935865670.9119373200610.6152767446456591326 04.985314307367ImpurityWeak
8	8.2898441106521810454.5061563472681.2512498472167635162721.00342231174ImpurityWeak
9	8.2026207684960334987.7430892958641.6354066501854287102636.44725478534ImpurityWeak
10	8.1451066926651752202 6.1839907193350.7867063506966306194328.25867914205ImpurityWeak
11	8.1435157751914974468 3.1724529396961.9984348659589595115426 0.7933839571ImpurityNone
12	8.1370717917633995664.19974135960.7620892612457261416 93.0785257779ImpurityWeak
13	8.1346313611116464563 0.357860596721.4153714783838327834744.7002039717ImpurityNone
14	8.1328899478570473416 8.47877846041.1189903151311364880 40.3086913662ImpurityWeak
15	8.1070876772081674387.7288506071090.8998562782244879382 05.51533841462ImpurityWeak
16	8.0972828526807922145 6.933248528480.8549948003364081191 043.98177346063ImpurityWeak
17	8.0956755034870763802 2.818365726111.7882764486184159069 90.5086726755CompoundNone
18	8.0871346773778361440 91.684790327971.1229203929768672205 8215.9710538494CompoundNone
19	8.0851439945950662739 0.5562496625641.0670702849935763415 832.4183604857CompoundNone
20	8.0687148967451538782.9535659214453.9420513570279683252 16.3401044855ImpurityWeak
21	8.0582778166824866116.2411071933361.9270437313352478157624.8060740803ImpurityWeak
22	8.0262225772635374920 9.016972046220.8744253100912436461369.5393665215ImpurityNone
23	8.0246397822545738145 4.190748749461.5611569321452126161707 1.4491185073ImpurityNone
24	8.0226504846489811380 8.784939193641.2695120355714211191625.03201476784ImpurityWeak

Topspin: csv, many columns
`process_peaks(method = "Topspin")`



	A	B	C	D
	Peak	v(F1) [ppm]	Intensity [abs]	Annotation
1	1	8.4432	165808.94	
2	2	7.8655	53795.69	
3	3	7.8638	56153.72	
4	4	7.4168	89039.75	
5	5	7.4141	90839.69	
6	6	7.4054	80783.56	
7	7	7.3982	59240.28	
8	8	7.3901	54182.12	
9	9	7.3847	52922.19	
10	10	7.381	58258.09	
11	11	7.3732	65480.06	
12	12	7.3678	67829.69	
13	13	7.3601	67041.28	
14	14	7.3477	54136.72	

`compute_relabund_cores(method = "peaks")`
Add the "area" values within each bin.
Calculates relative abundance for each sample.

[Topspin file has "intensity" column, not "area", current workaround is to rename intensity to area (lazy way out, quicker than making a new if loop).

`compute_relabund_treatment()`
From sample-level relative abundance, computes averages by treatment. Good for summary tables, stacked bar plots, etc.