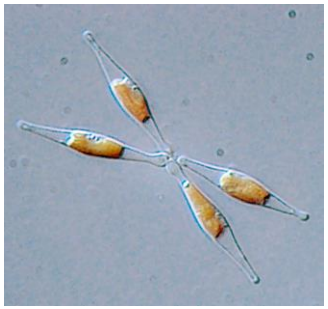
Titre du projet : Apport de la métabolomique dans l'identification des facteurs de transcription régulant l'accumulation de lipides par les microalgues au cours d'un stress

Auteurs: *Florence Mondeguer, Manoella Sibat Laboratoire PHYCOTOXINES, Ifremer, Nantes*
Justine Marchand, Laboratoire MMS, Le Mans Université, Equipe MIMMA

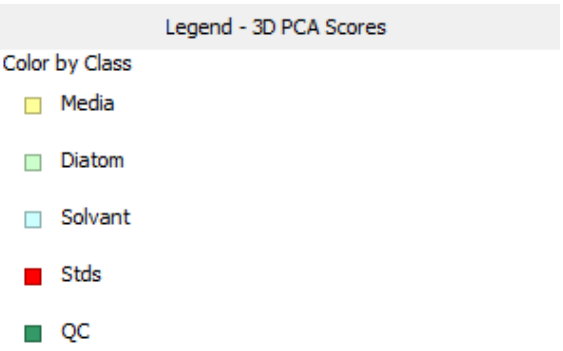


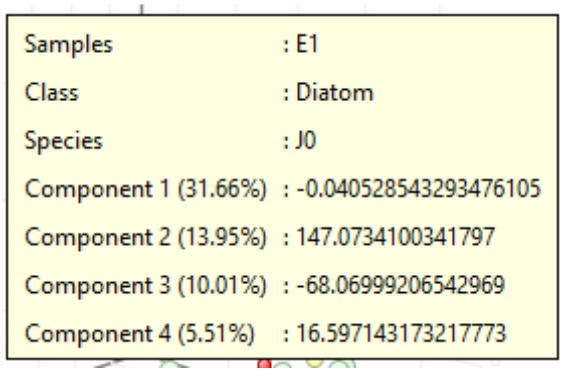
Résumé du projet :

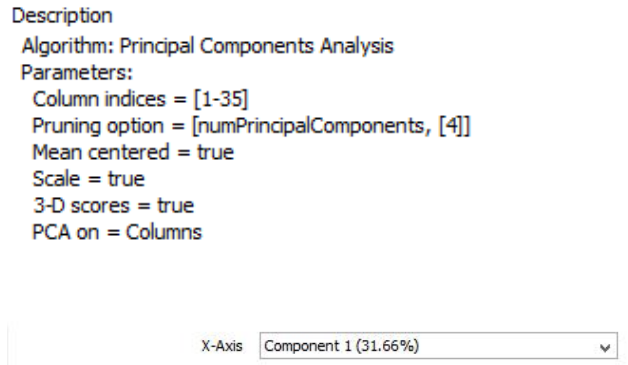
Des expériences de culture (photobioréacteurs) de Phaeodactylum tricornutum, en condition de carence en azote, (favorisant la production de lipides ont été réalisés au laboratoire MMS. Le suivit physiologique et biochimique des cultures ainsi qu'une analyse transcriptomique (expression différentielle des gènes) permet de s'intéresser aux facteurs de transcription impliqués dans le contrôle de la voie de biosynthèse des lipides et des pigments chez cette diatomée. L'objectif du projet est de compléter cette étude par une approche métabolomique qui permettra d'identifier de façon globale l'ensemble des métabolites différentiellement formés permettant ainsi, associée à l'étude des gènes (transcriptomique), d'obtenir une vision intégrée de l'orientation des atomes de carbone dans les différentes voies de biosynthèse.

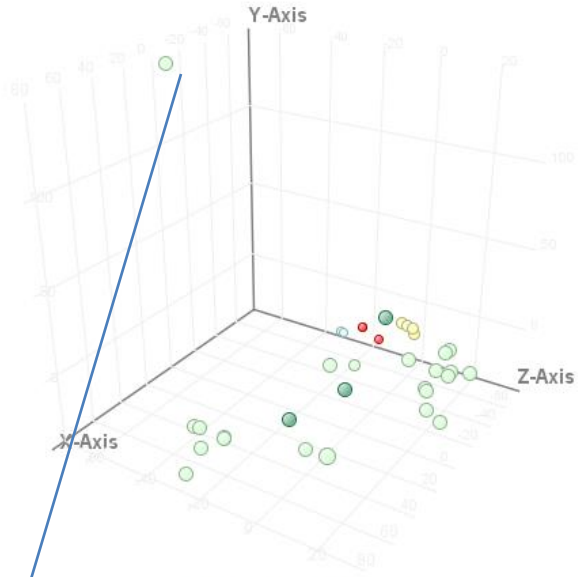
MassProfilerProfessional reprocessing

Quality control on samples







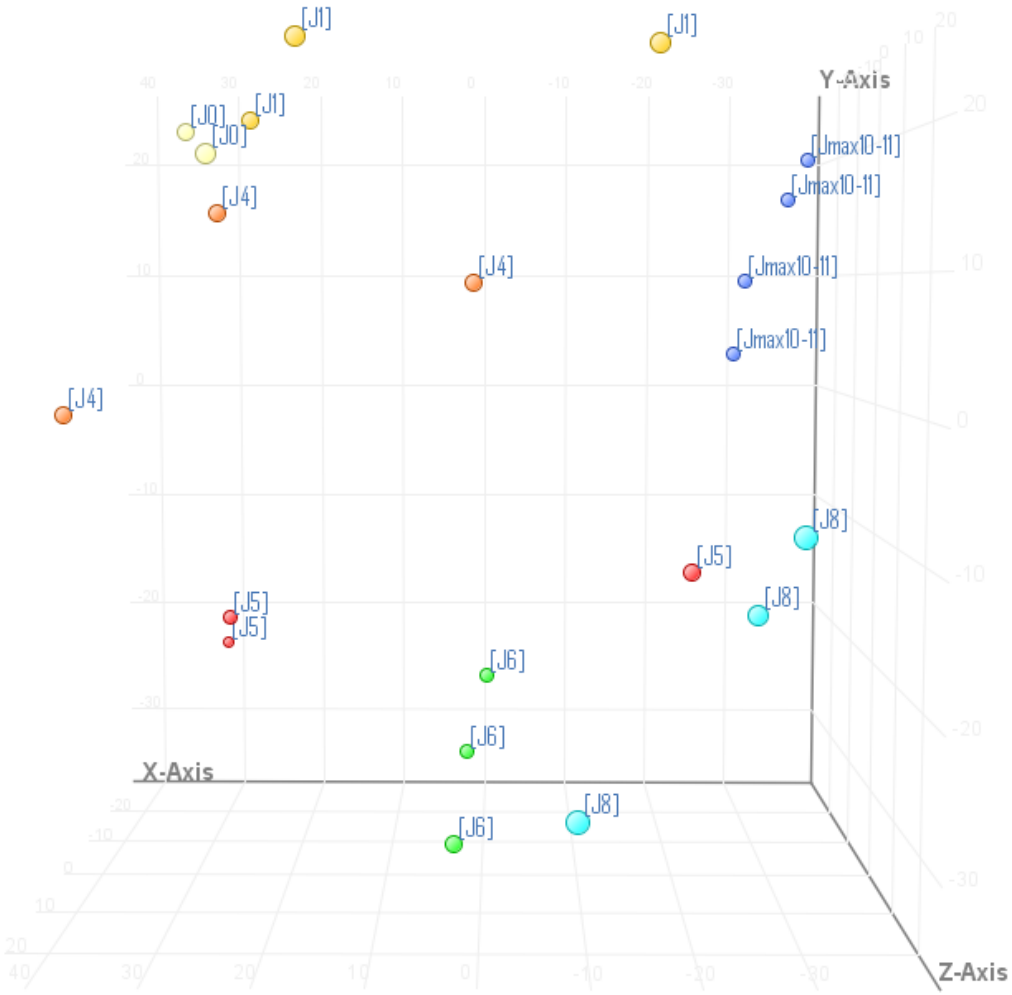


Outlier ?

Ce premier échantilon a- t-il subit une pression particulière?

Ni non ce n'est pas très grave on peut le garder…

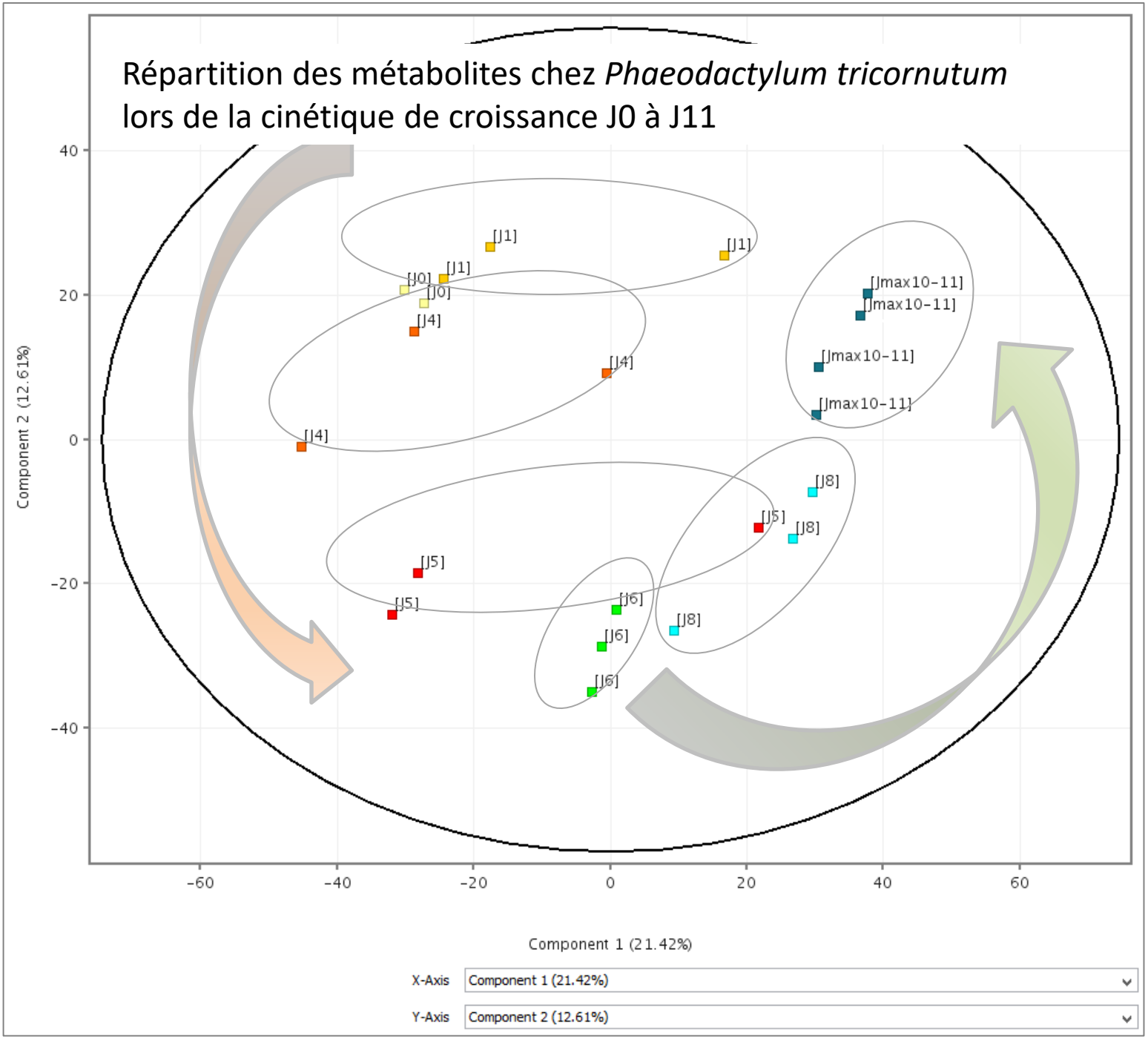
A décider



X-Axis Component 1 (21.53%) Y-Axis Component 2 (12.63%) Z-Axis Component 3 (8.41%)

PCA Loadings | C-C Plot | Eigenvalues | PCA Scores | 3D PCA Scores

Répartition des métabolites chez *Phaeodactylum tricornutum* lors de la cinétique de croissance J0 à J11

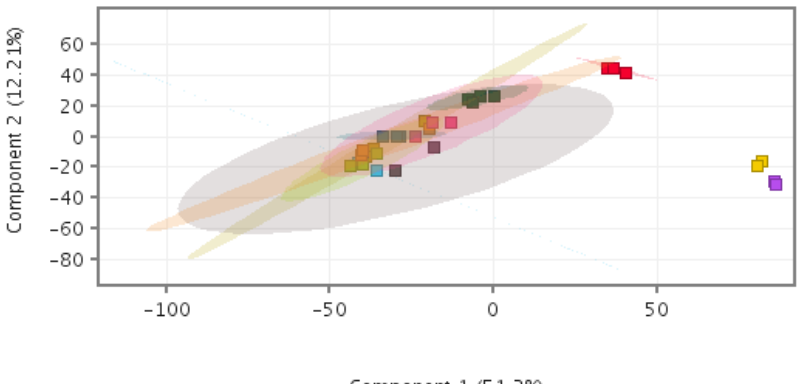


3D ACP ts samples

PCA (Step 3 of 4)

Output views

Output views of PCA. PCA on Entities; Entities with high scores for a particular PCA component follow the expression pattern shown in the PCA Loadings plot and can be selected to be saved as custom lists. PCA on Conditions; Samples with similar scores for one or more PCA components can be considered similar in their expression profile.



X-Axis: Component 1 (51.2%)

Y-Axis: Component 2 (12.21%)

Eigenvalues | PCA Scores | 3D PCA Scores | PCA Loadings | C-C Plot

Legend - PCA Scores

Color by Species

- Blank
- CTRL
- J0
- J1
- J4
- J5
- J6
- J8
- Jmax10-11
- Meoh
- Stds

Description

Algorithm: Principal Components Analysis
Parameters:
Column indices = [1-34]
Pruning option = [numPrincipalComponents, [4]]
Mean centered = true
Scale = true

Save custom list...

Help | << Back | Next >> | Finish | Cancel

PCA (Step 1 of 4)

Entity List and Interpretation.

Principal Components Analysis (PCA) allows for the detection of major trends in your data. Choose the entity list and interpretation.

Entity List: 4113-Fold change >= 2.0 — Choose...

Interpretation: Species (Non-averaged) — Choose...

Help | << Back | Next >> | Finish | Cancel

PCA (Step 2 of 4)

Input Parameters

PCA on Entities allows for the detection of those entities that most prominently define the major trends in the data, PCA on conditions allows for the detection of similarity between samples, discriminated by the major trends in the data. Choose the number of principal components or choose the percentage of variation you want them to explain.

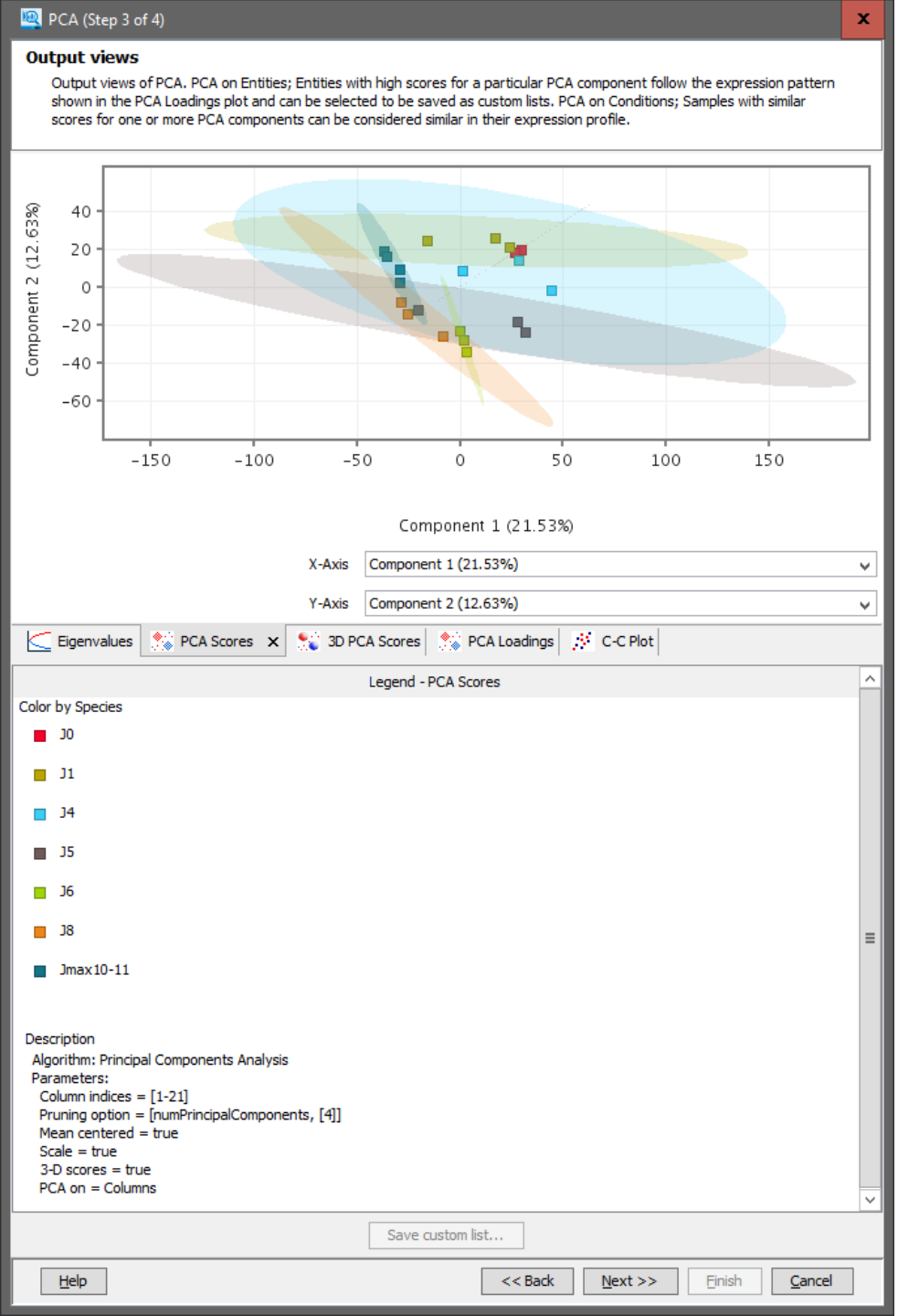
PCA on: Conditions

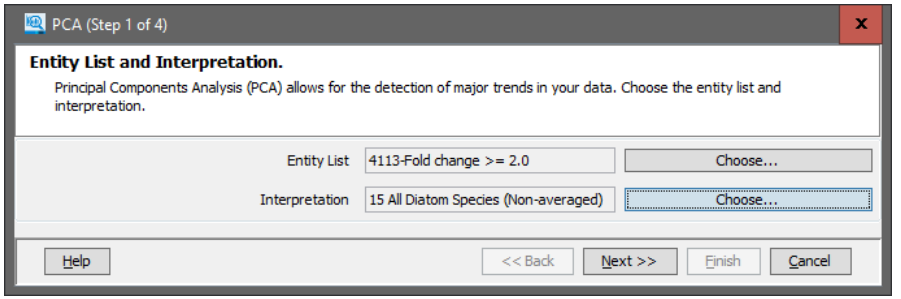
Pruning option

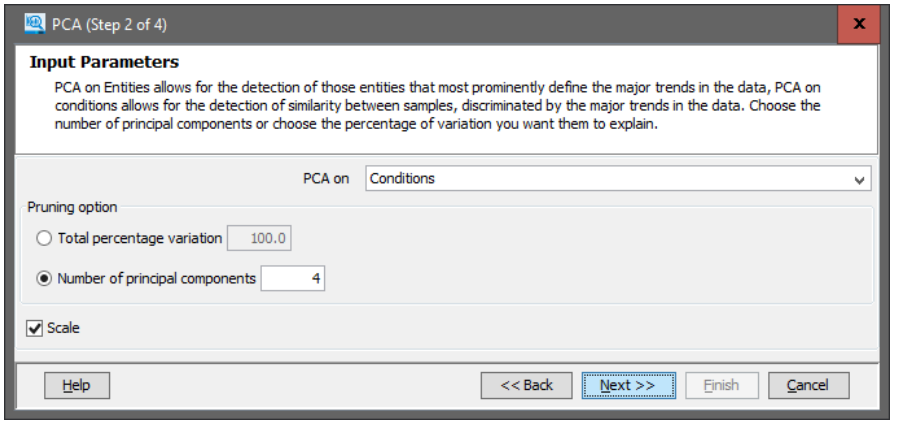
- Total percentage variation: 100.0
- Number of principal components: 4

Scale

Help | << Back | Next >> | Finish | Cancel

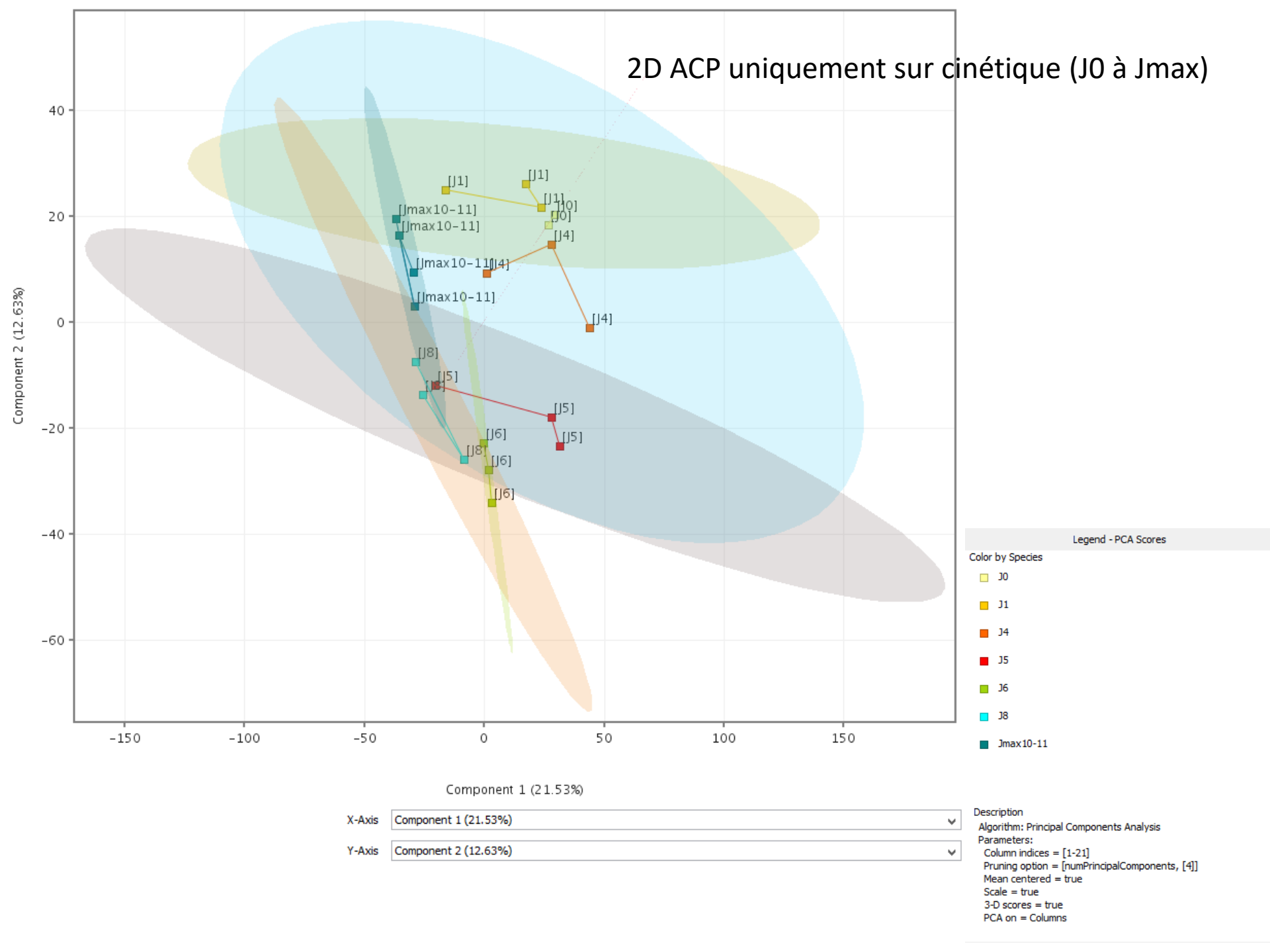


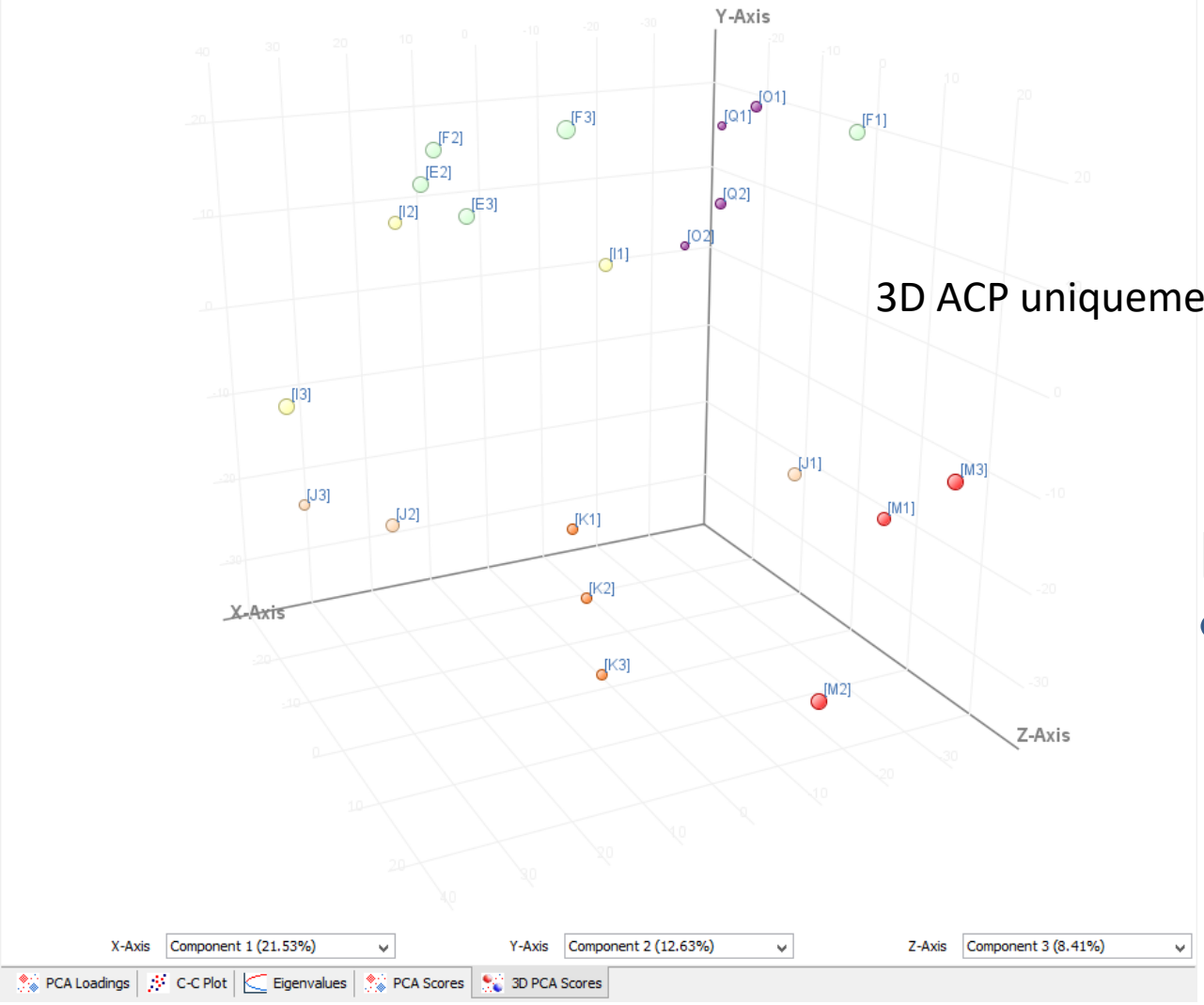




3D ACP uniquement sur cinétique (J0 à Jmax)

2D ACP uniquement sur cinétique (J0 à Jmax)





Comme demandé essai avec J0et J1 cumulés

3D ACP uniquement sur cinétique (J0 à Jmax)

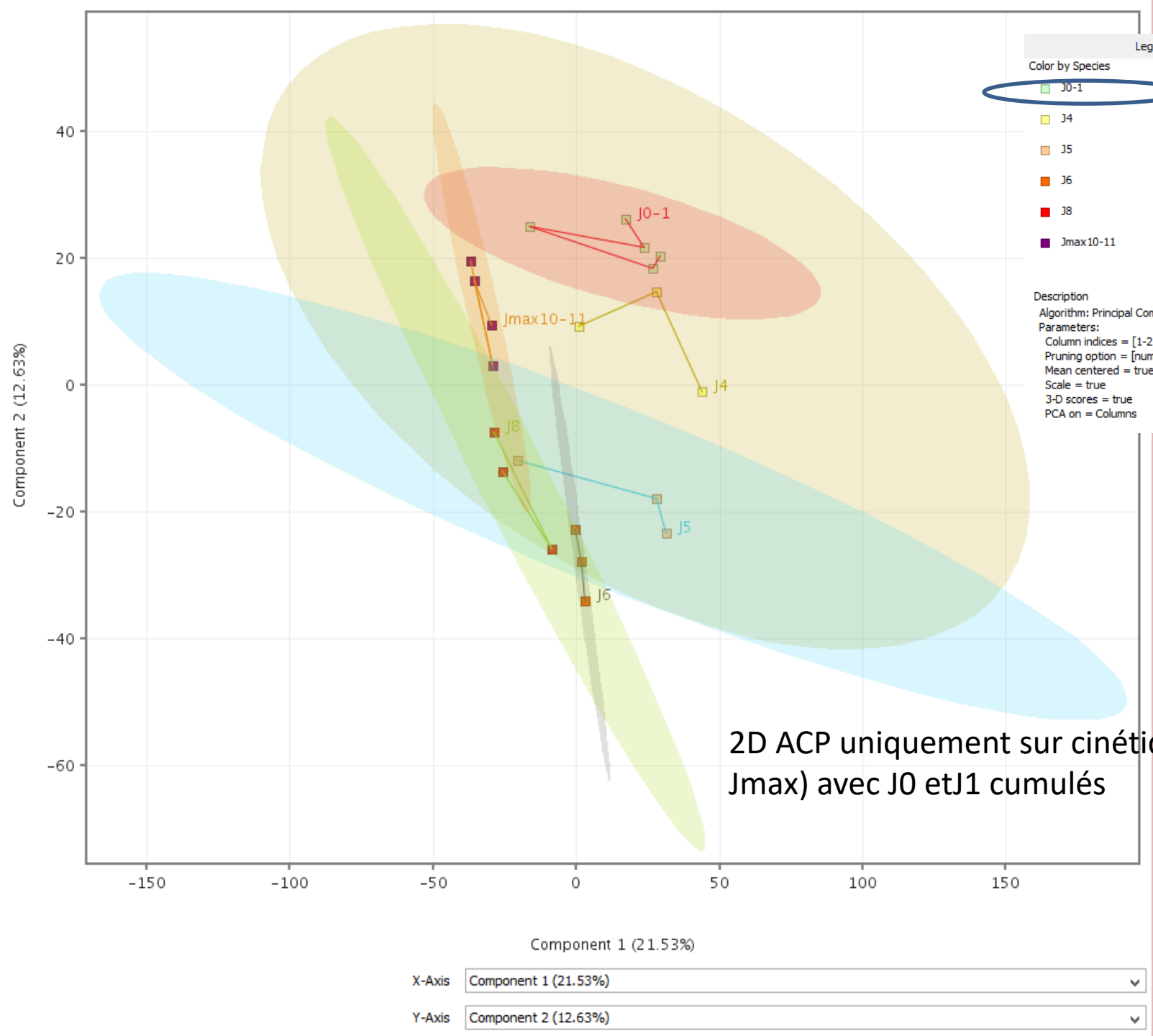
Legend - 3D PCA Scores

Color by Species

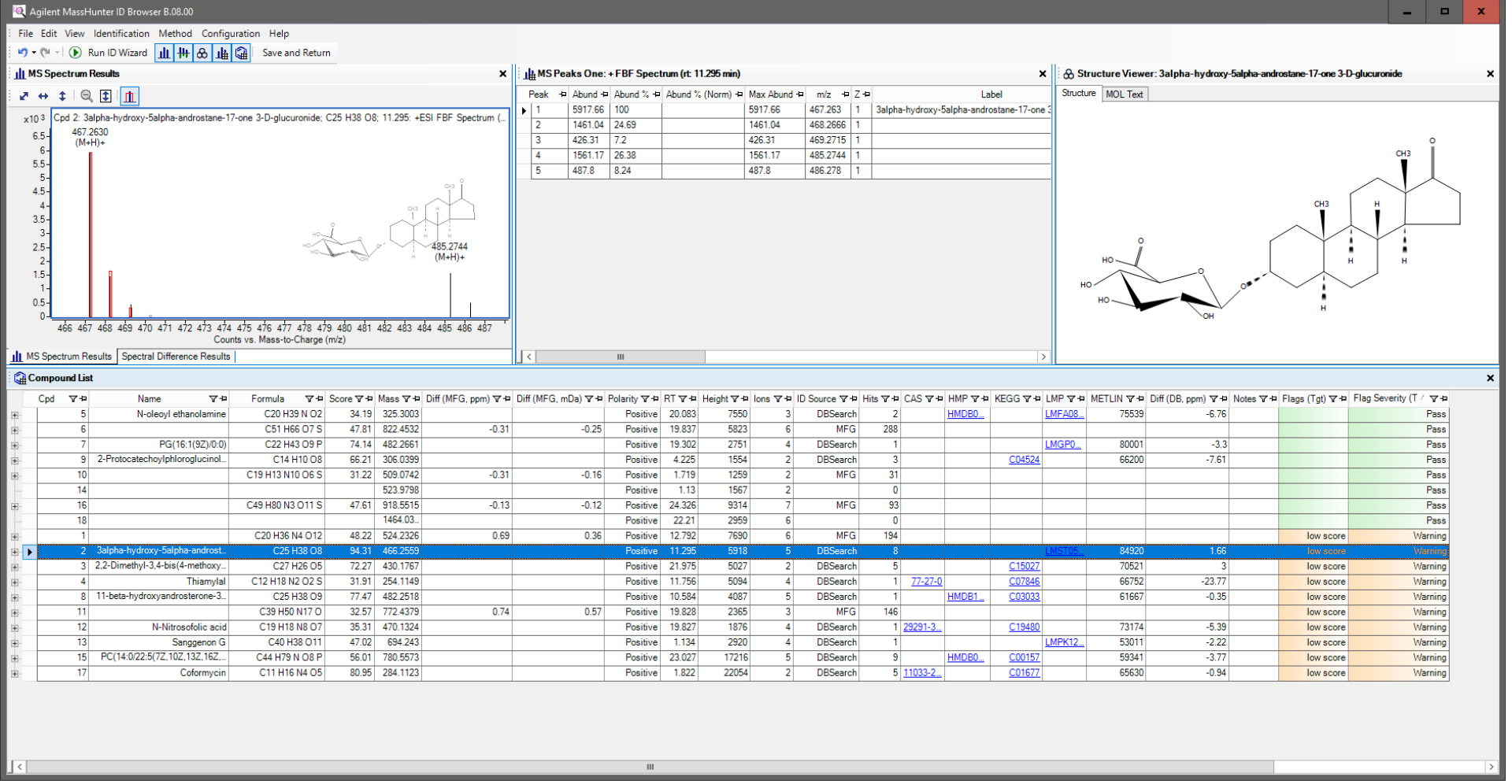
- J0-1
- J4
- J5
- J6
- J8
- Jmax10-11

Description

Algorithm: Principal Components Analysis
Parameters:
Column indices = [1-21]
Pruning option = [numPrincipalComponents, [3]]
Mean centered = true
Scale = true
3-D scores = true
PCA on = Columns



2D ACP uniquement sur cinétique (J0 à Jmax) avec J0 etJ1 cumulés



Secondary metabolite identification for 18 Entities unic J0:

Best Know: 3/18

- Cpd 7: PG(16:1(9Z)/0:0); C22H43O9P@19.302 Score: 74.14

PG(16:1(9Z)/0:0) is a lysophosphatidylglycerol 16:1.

lyso-PG (16:1) :Changes of lipid molecular species during cold stress

…..next slide

Secondary metabolite identification for 18 Entities unic J0:
Best Know: 3/18

- Cpd 7: PG(16:1(9Z)/0:0); C22H43O9P@19.302 Score: 74.14

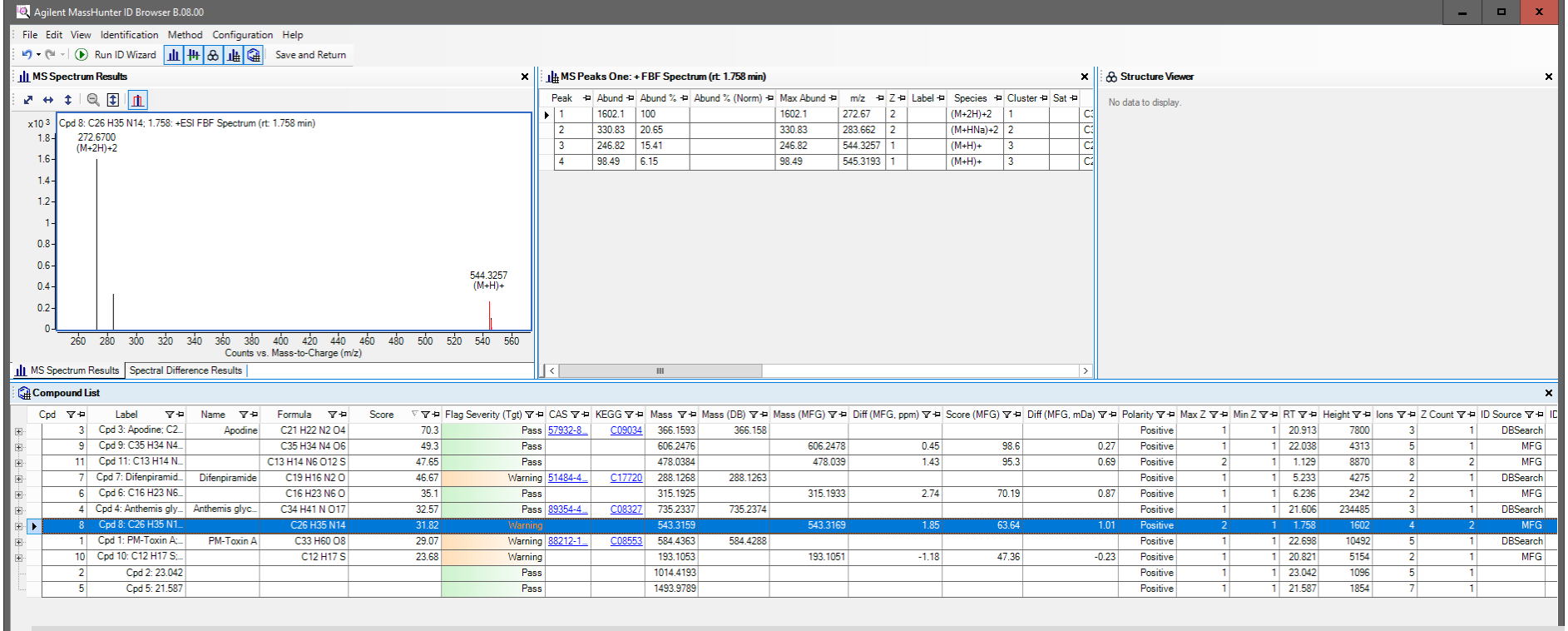
PG(16:1(9Z)/0:0) is a lysophosphatidylglycerol 16:1.
lyso-PG (16:1) :Changes of lipid molecular species during cold stress

- Cpd 9: 2-Protocatechoylphloroglucinolcarboxylate; C14H10O8@4.225 score: 66.21

2-Protocatechoylphloroglucinolcarboxylate= **2-(3,4-Dihydroxybenzoyloxy)-4,6-dihydroxybenzoate**: A metabolite of quercetin, an abundant flavonoid found in edible vegetables, grains and fruits which is used as an ingredient in supplements, beverages, or foods. It is a dihydroxybenzoic acid and a benzoate ester. It is a conjugate acid of a 2-(3,4-dihydroxybenzoyloxy)-4,6-dihydroxybenzoate.

- Cpd 5: N-oleoyl ethanolamine; C20H39NO2@20.083 score:34.19

Oleoylethanolamide (OEA or NOE) is an N-acylethanolamine.
N-Acylethanolamines (NAEs) constitute a class of lipid compounds naturally present in both animal and plant membranes as constituents of the membrane-bound phospholipid,



Secondary metabolite identification for 11 Entities unic J1:

Best Know: 1/11 (mais 2 choix)

Cpd 3: Octocrylene; C24H27NO2@20.913,Octocrylene Score:78.28

Octocrylene is an organic compound used as an ingredient in sunscreens and cosmetics?

Autre possibilité avec un score légèrement plus petit si aucune contamination n'est envisageable alors:

Cpd 3: Apodine;C21H22N2O4 @20.913 Score:70.3

Phytochemical compounds Alkaloids

Some of the allelopathic compounds from algae and seaweeds have been isolated and characterized including alkaloids and marine diatom *Phaeodactylum tricornutum* is known to exude allelochemicals with negative effects.

Secondary metabolite identification for 9 Entities unic J4 :

Best Know: 3/9

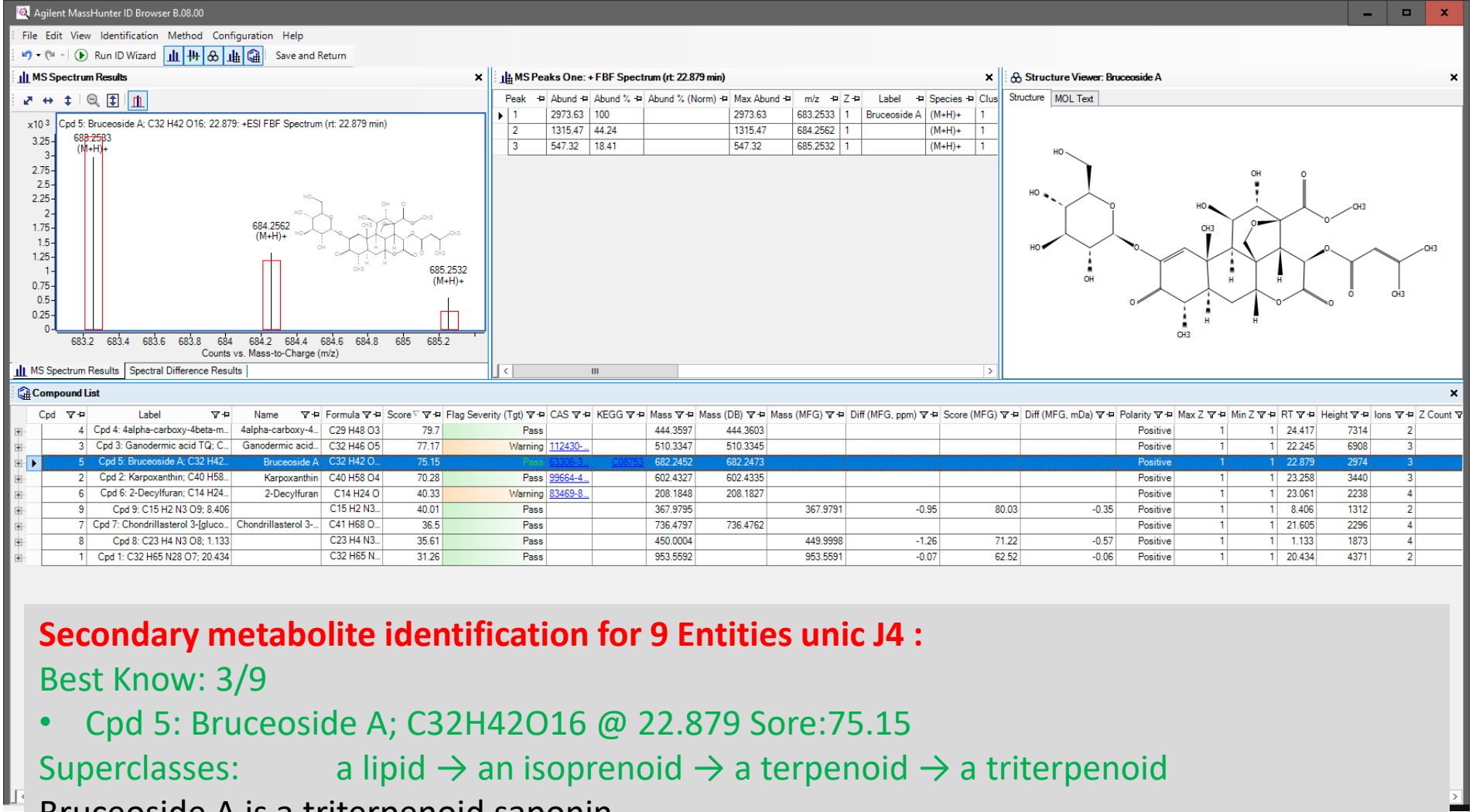
- Cpd 4: 4alpha-carboxy-4beta-methyl-5alpha-cholesta-8-en-3beta-ol OR 3β-hydroxysteroid-4α-carboxylate; C29H48O3 @24.417 Score:79.7

cholesterol biosynthesis II (via 24,25-dihydrolanosterol).

Superclasses: a steroid → a hydroxysteroid → a sterol → a 3beta-hydroxysteroid

Steroids are abundant in the environment. Large amounts of steroids and their derivatives are synthesized by eukaryotes, and these molecules play very important and diverse roles and include hormones, detergents that facilitate the absorption of lipids by the intestine, and membrane constituents. Some of them, cholesterol and related compounds, are ubiquitous as membrane constituent of eukaryotes (for instance, up to 10% of the dry mass of yeast is ergosterol) and as the precursors of all steroid hormones, vitamin D, and the bile acids.

Interestingly, with exception of methane-oxidizing bacteria that contain relatively large amounts of sterols, sterols are absent from most prokaryotes. However, many bacterial membranes contain hopanoids, which are similar pentacyclic sterol-like molecules [Chiang08].



Secondary metabolite identification for 9 Entities unic J4 :

Best Know: 3/9

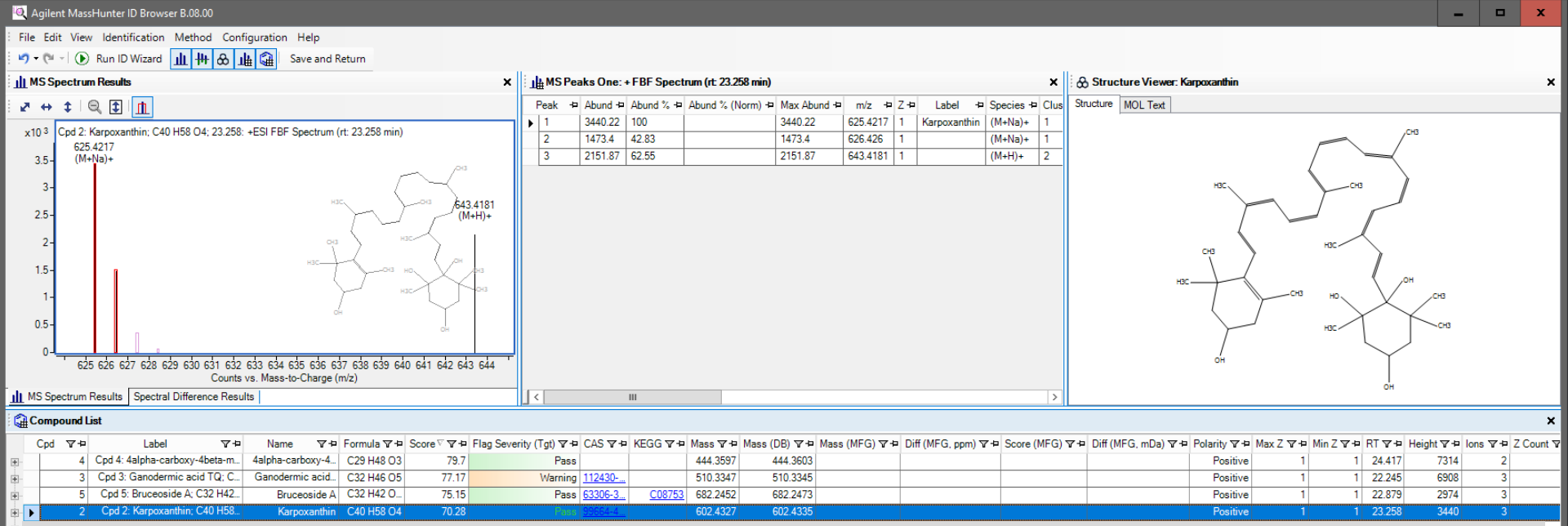
- Cpd 5: Bruceoside A; C32H42O16 @ 22.879 Sore:75.15

Superclasses: a lipid → an isoprenoid → a terpenoid → a triterpenoid

Bruceoside A is a triterpenoid saponin

Plant triterpenoids constitute a diverse class of organic compounds that play a major role in development, plant defence and environmental interaction. Several triterpenes have demonstrated potential as pharmaceuticals.

For example, some have reported the production of the triterpenes betulin and its precursor lupeol in the photosynthetic diatom *Phaeodactylum tricornutum*



Secondary metabolite identification for 9 Entities unic J4 :

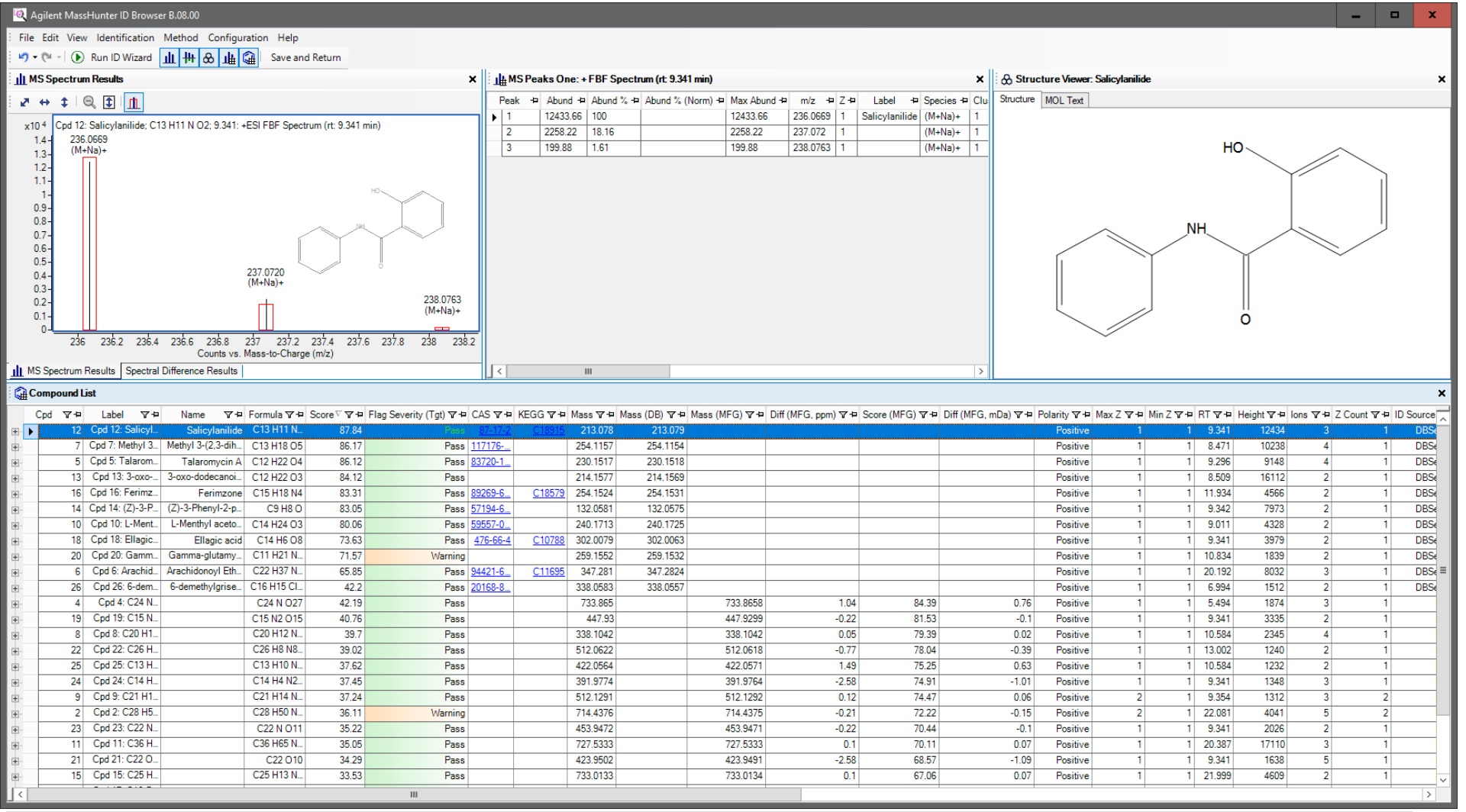
Best Know: 3/9

- Cpd 2: Karpoxanthin; C40H58O4@23.258 Score 70.28

Furthermore, annually, more than 20 new structures of carotenoids are reported ...

from diatom Phaeodactylum tricornutum (Photosynthetic pigments in diatoms. P Kuczynska, M Jemiola-Rzeminska, K Strzalka - Marine drugs, 2015 - mdpi.com)

Carotenoids are C40 isoprenoids which consist of eight isoprene units and can be divided in two major groups: carotenes and xanthophylls. Carotenes are linear or cyclized hydrocarbons such as lycopene, α-carotene and β-carotene. Xanthophylls are oxygenated derivatives (epoxy, keto or hydroxyl groups) of carotenes; for example: lutein and zeaxanthin. The carotenoid composition varies from species to species; the concentration and composition of xanthophylls are affected by light intensity and the accumulation of specific carotenoids in fruit and flower chromoplasts is a highly, developmentally regulated process [Fraser94, Giuliano93]. Important carotenoids variations are observed during fruit ripening (for review, see [Ronen99]). Higher plant chloroplasts typically accumulate lutein, β-carotene, violaxanthin and neoxanthin in the thylakoid membrane-bound photosystems [Peter91, Ryberg93]. β-Carotene is generally found in the reaction center where it plays a critical photoprotective role by quenching triplet chlorophyll and singlet oxygen, and can undergo rapid degradation during photooxidation [Young93a]. Adjacent to the reaction centers, in the core complex proteins, β-carotene and lutein can be found [Peter91, Bassi93]. Finally, the surrounding antenna complexes contain xanthophylls (lutein, violaxanthin and neoxanthin) [Peter91, Bassi93]. In the chromoplasts of ripening fruits and flower petals, and in the chloroplasts of senescing leaves, the carotenoids are found in membranes or in oil bodies or other structures within the stroma.



Secondary metabolite identification for 26 Entities unic J5:

J5 semble une étape cruciale dans la croissance de Phaeodactylum on détecte 26 composés spécifiques à cette étapes dont:

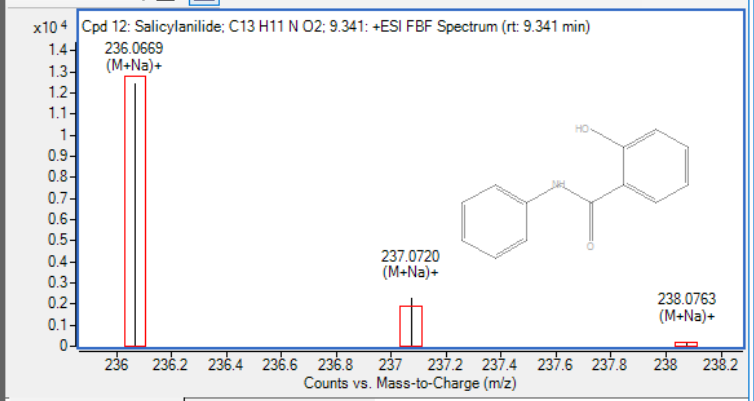
Best Know: 9/926

Agilent MassHunter ID Browser B.08.00

File Edit View Identification Method Configuration Help

Run ID Wizard | Save and Return

MS Spectrum Results



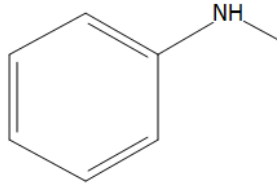
MS Spectrum Results | Spectral Difference Results

MS Peaks One: + FBF Spectrum (rt: 9.341 min)

Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label	Species	Clu
1	12433.66	100		12433.66	236.0669	1	Salicylanilide	(M+Na)+	1
2	2258.22	18.16		2258.22	237.072	1		(M+Na)+	1
3	199.88	1.61		199.88	238.0763	1		(M+Na)+	1

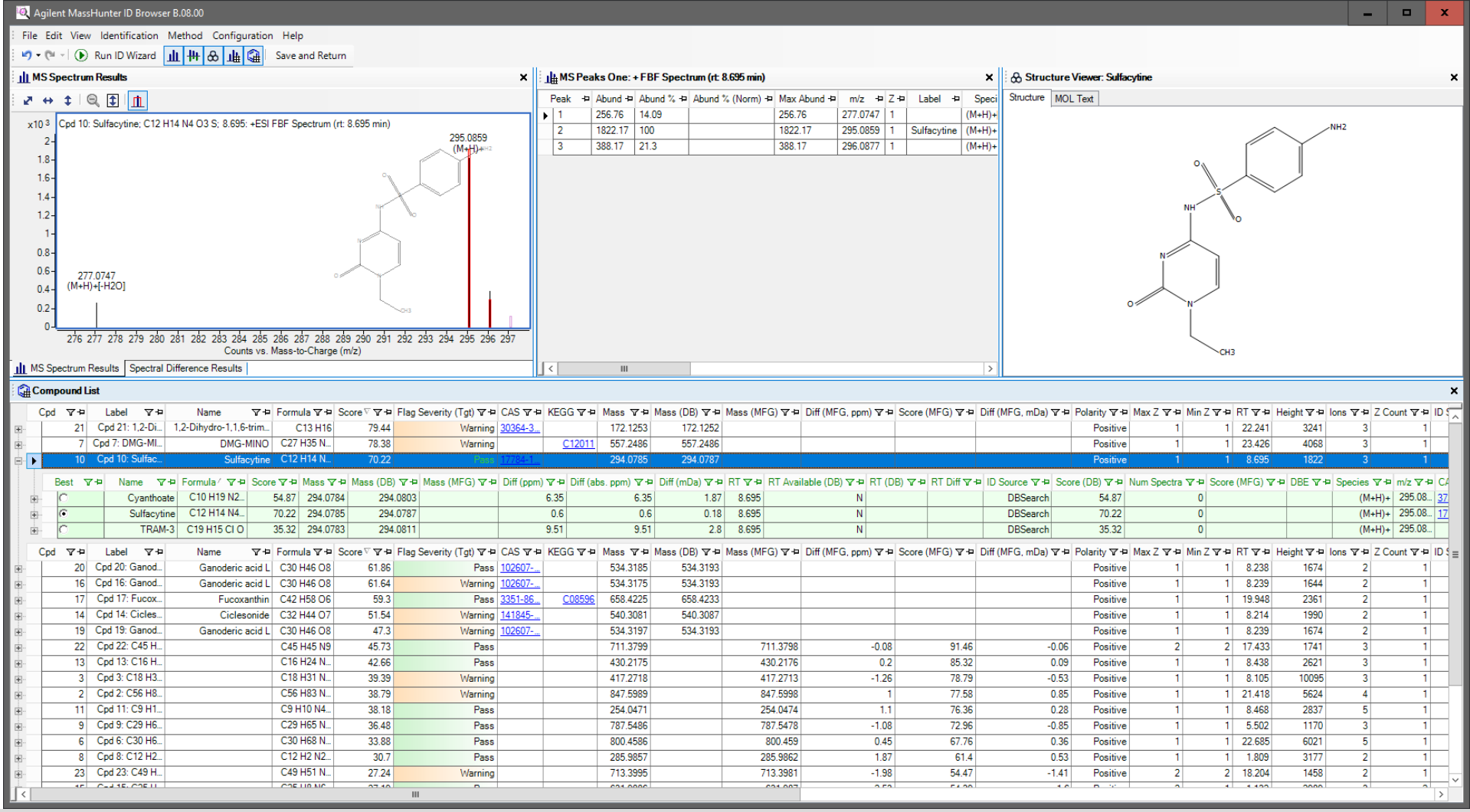
Structure Viewer: Salicylanilide

Structure | MOL Text



Compound List

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	RT
12	Cpd 12: Salicyl...	Salicylanilide	C13 H11 N...	87.84	Pass	87-17-2	C18515	213.078	213.079					Positive	1	1	9.34
7	Cpd 7: Methyl 3...	Methyl 3-(2,3-dih...	C13 H18 O5	86.17	Pass	117176-...		254.1157	254.1154					Positive	1	1	8.47
5	Cpd 5: Talarom...	Talaromycin A	C12 H22 O4	86.12	Pass	83720-1...		230.1517	230.1518					Positive	1	1	9.29
13	Cpd 13: 3-oxo-...	3-oxo-dodecanoi...	C12 H22 O3	84.12	Pass			214.1577	214.1569					Positive	1	1	8.50
16	Cpd 16: Ferimz...	Ferimzone	C15 H18 N4	83.31	Pass	89269-6...	C18579	254.1524	254.1531					Positive	1	1	11.93
14	Cpd 14: (Z)-3-P...	(Z)-3-Phenyl-2-p...	C9 H8 O	83.05	Pass	57194-6...		132.0581	132.0575					Positive	1	1	9.34
10	Cpd 10: L-Ment...	L-Menthyl aceto...	C14 H24 O3	80.06	Pass	59557-0...		240.1713	240.1725					Positive	1	1	9.01
18	Cpd 18: Ellagic...	Ellagic acid	C14 H6 O8	73.63	Pass	476-66-4	C10788	302.0079	302.0063					Positive	1	1	9.34
20	Cpd 20: Gamm...	Gamma-glutamy...	C11 H21 N...	71.57	Warning			259.1552	259.1532					Positive	1	1	10.83
6	Cpd 6: Arachid...	Arachidonoyl Eth...	C22 H37 N...	65.85	Pass	94421-6...	C11695	347.281	347.2824					Positive	1	1	20.19
26	Cpd 26: 6-dem...	6-demethylgrise...	C16 H15 Cl...	42.2	Pass	20168-8...		338.0583	338.0557					Positive	1	1	6.99
4	Cpd 4: C24 N...		C24 N O27	42.19	Pass			733.865		733.8658	1.04	84.39	0.76	Positive	1	1	5.49
19	Cpd 19: C15 N...		C15 N2 O15	40.76	Pass			447.93		447.9299	-0.22	81.53	-0.1	Positive	1	1	9.34
8	Cpd 8: C20 H1...		C20 H12 N...	39.7	Pass			338.1042		338.1042	0.05	79.39	0.02	Positive	1	1	10.58
22	Cpd 22: C26 H...		C26 H8 N8...	39.02	Pass			512.0622		512.0618	-0.77	78.04	-0.39	Positive	1	1	13.00
25	Cpd 25: C13 H...		C13 H10 N...	37.62	Pass			422.0564		422.0571	1.49	75.25	0.63	Positive	1	1	10.58
24	Cpd 24: C14 H...		C14 H4 N2...	37.45	Pass			391.9774		391.9764	-2.58	74.91	-1.01	Positive	1	1	9.34
9	Cpd 9: C21 H1...		C21 H14 N...	37.24	Pass			512.1291		512.1292	0.12	74.47	0.06	Positive	2	1	9.35
2	Cpd 2: C28 H5...		C28 H50 N...	36.11	Warning			714.4376		714.4375	-0.21	72.22	-0.15	Positive	2	1	22.08
23	Cpd 23: C22 N...		C22 N O11	35.22	Pass			453.9472		453.9471	-0.22	70.44	-0.1	Positive	1	1	9.34
11	Cpd 11: C36 H...		C36 H65 N...	35.05	Pass			727.5333		727.5333	0.1	70.11	0.07	Positive	1	1	20.38
21	Cpd 21: C22 O...		C22 O10	34.29	Pass			423.9502		423.9491	-2.58	68.57	-1.09	Positive	1	1	9.34
15	Cpd 15: C25 H...		C25 H13 N...	33.53	Pass			733.0133		733.0134	0.1	67.06	0.07	Positive	1	1	21.99

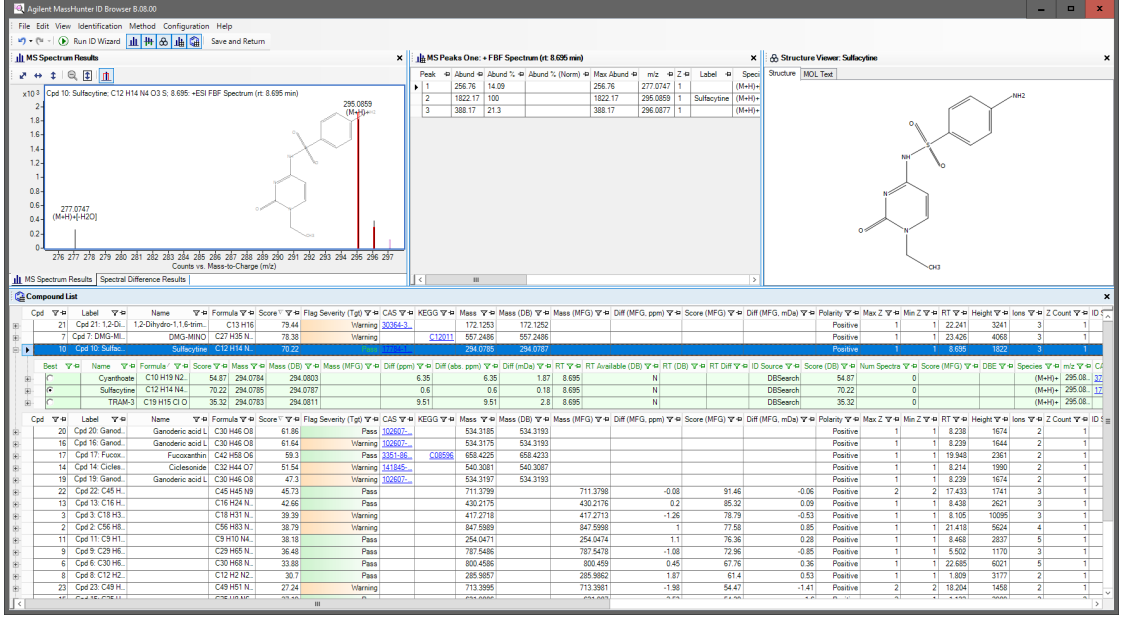


Secondary metabolite identification for 23 Entities unic J6:

J6 semble être une autre étape cruciale dans la croissance de Phaeodactylum proche de J5 et pour laquelle on détecte 23 composés spécifiques mais dont l'identification se résume à 1 ou 2 composés pour lequel l'identification donne un score acceptable

Best Know: 2/23

- Cpd 10: Sulfacytine; C12H14N4O3S @8.695 Score: 70.22



Secondary metabolite identification for 23 Entities unic J6:

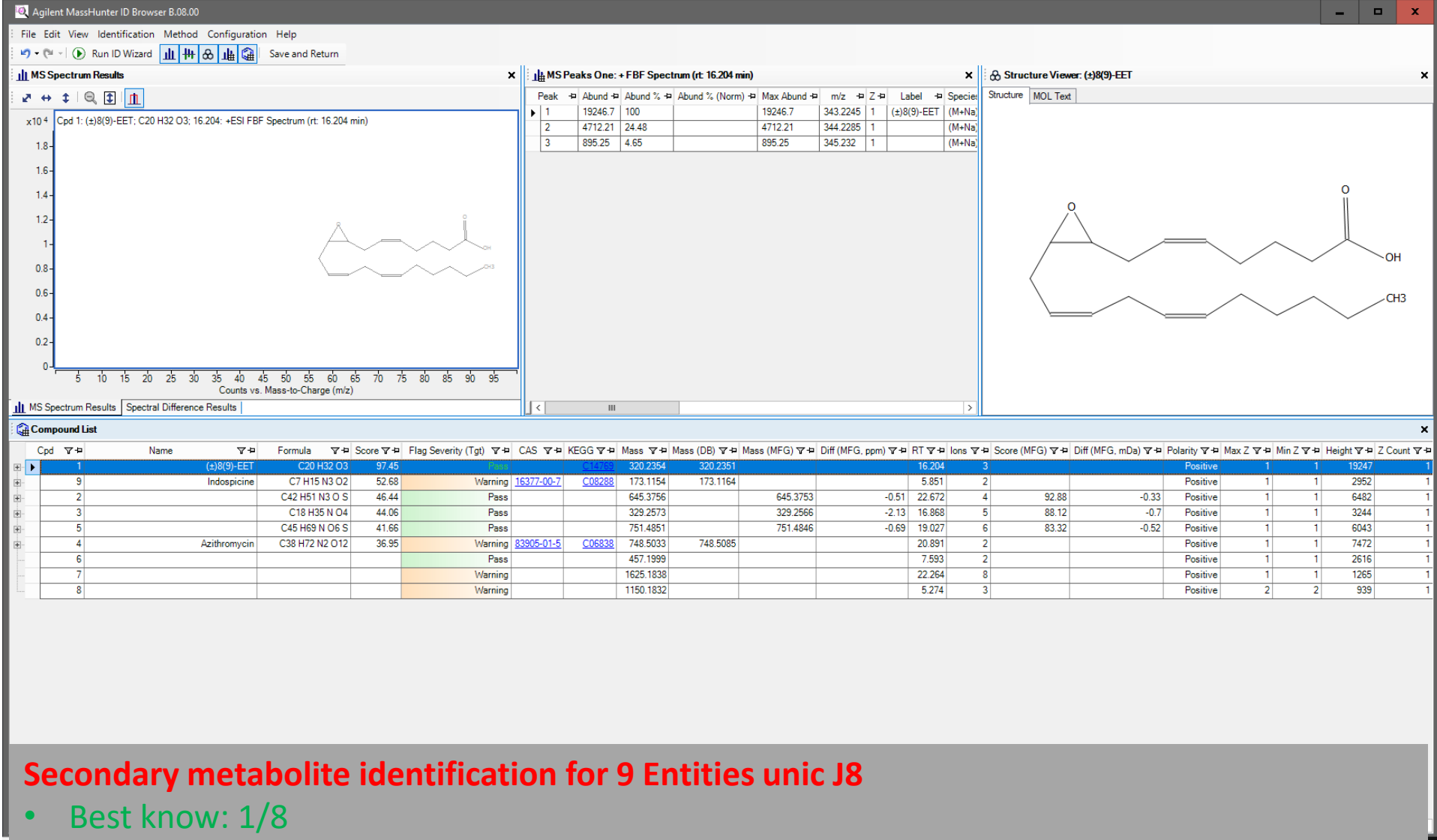
Best Know: 2/23

- Cpd 10: Sulfacytine; C12H14N4O3S @8.695 Score: 70.22

Sulfacytine is a member of benzenes and a sulfonamide. Sulfacytine is a short-acting, broad-spectrum sulfonamide and a synthetic analog of para-aminobenzoic acid (PABA) with bacteriostatic property. Sulfacytine competes with PABA for the bacterial enzyme dihydropteroate synthase, thereby preventing the incorporation of PABA into dihydrofolic acid, the immediate precursor of folic acid. This leads to an inhibition of bacterial folic acid synthesis and de novo synthesis of purines and pyrimidines, ultimately resulting in cell growth arrest and cell death

Cpd 20: Ganoderic acid L; C30H46O8 @8.238 Score: 61.86

There seems to exist certain relationship between specific Ganoderic acid production (ie content) and DOxygenT level. Further experiments were conducted to explore this potential Relationship (YJ Tang et al. 2003)



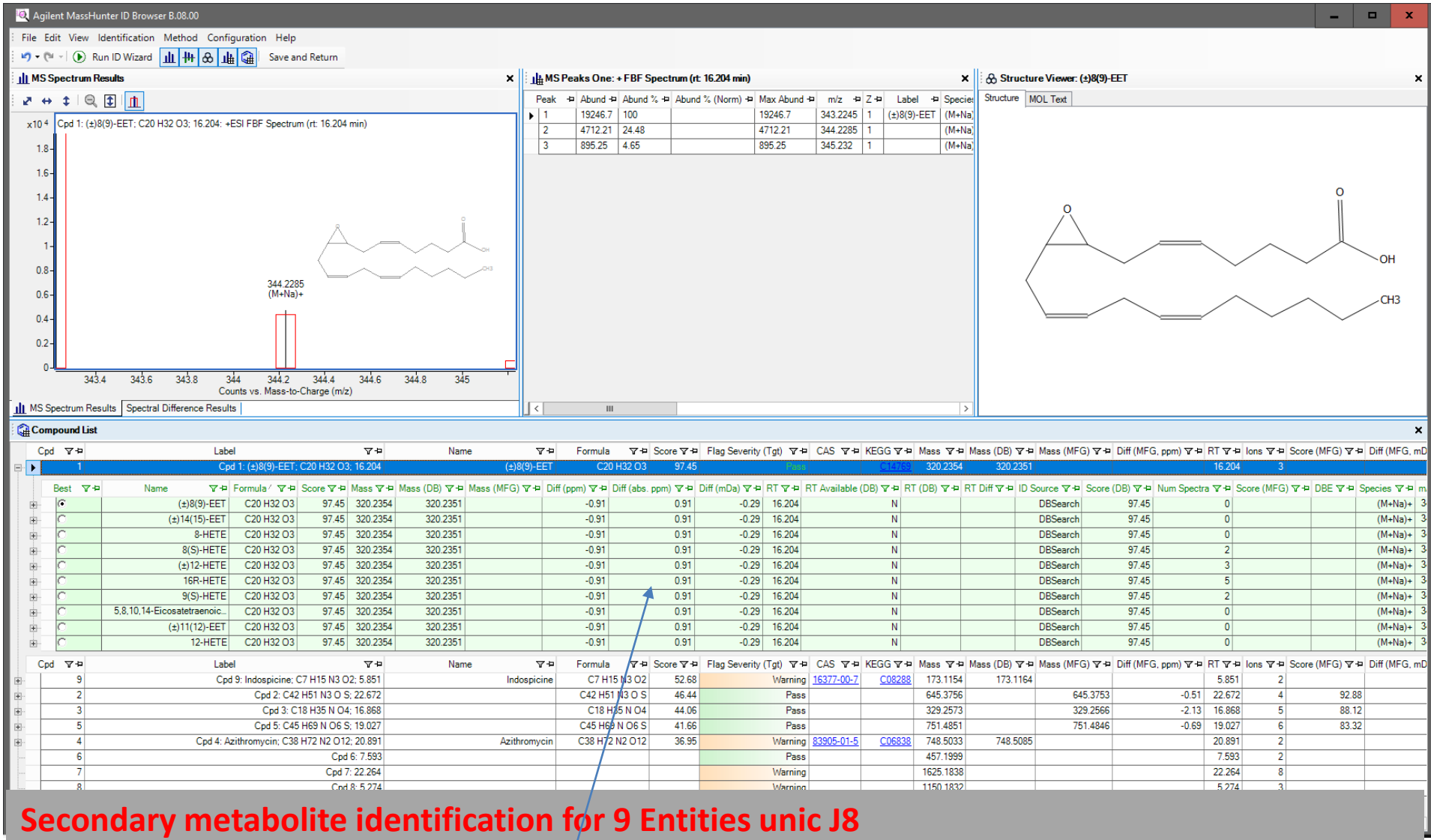
Secondary metabolite identification for 9 Entities unic J8

- Best know: 1/8

Oxylipin : eicosatetraenoic acid (5-HETE) ou bien 10 autres putatifs compounds visibles dans la slide suivante dans l'onglet en vert,

Cpd 1: (±)8(9)-EET; ; C20H32O3@16.204 score :97.45

Issu de: Arachidonic acid metabolism



Secondary metabolite identification for 9 Entities unic J8

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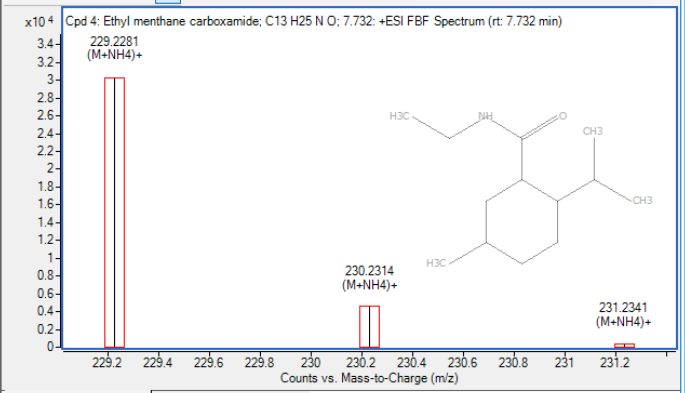
Issu de: Arachidonic acid metabolism

File Edit View Identification Method Configuration Help

Run ID Wizard | Save and Return

MS Spectrum Results



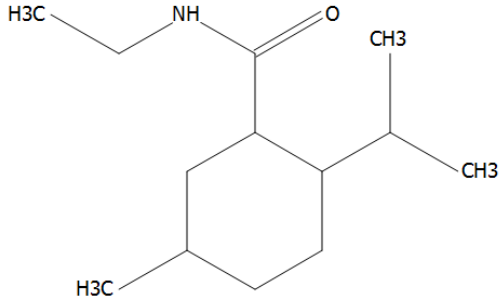
MS Spectrum Results | Spectral Difference Results

MS Peaks One: + FBF Spectrum (rt: 7.732 min)

Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label
1	30317.79	100		30317.79	229.2281	1	Ethyl menthane carb
2	4497.52	14.83		4497.52	230.2314	1	
3	372.87	1.23		372.87	231.2341	1	

Structure Viewer: Ethyl menthane carboxamide

Structure | MOL Text

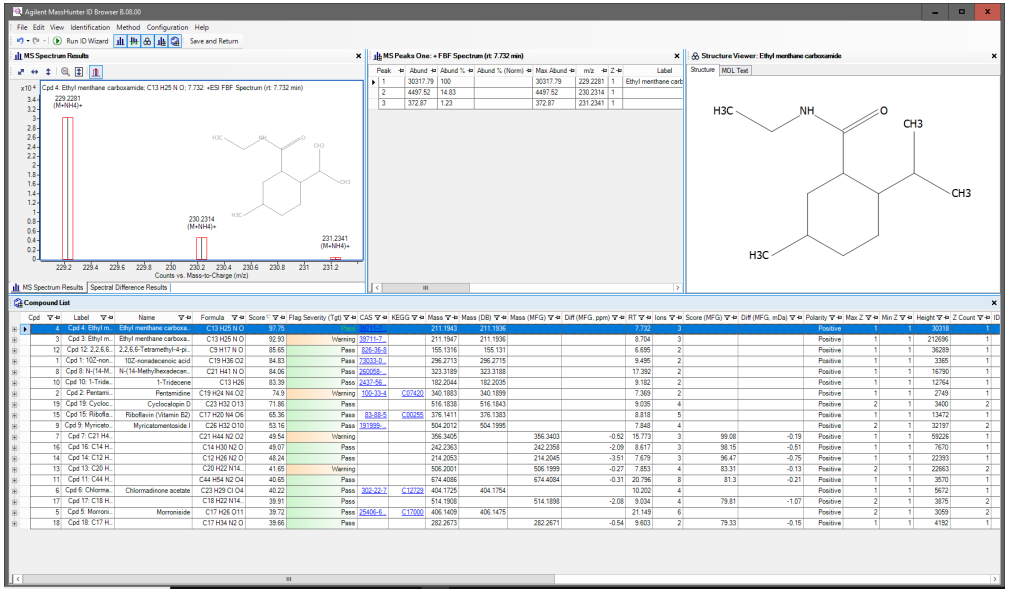


Compound List

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	RT	Ions	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	Height	Z Count	ID
4	Cpd 4: Ethyl m...	Ethyl menthane carboxa...	C13 H25 N O	97.75	Pass	39711-2...		211.1943	211.1936			7.732	3			Positive	1	1	30318	1	
3	Cpd 3: Ethyl m...	Ethyl menthane carboxa...	C13 H25 N O	92.93	Warning	39711-7...		211.1947	211.1936			8.704	3			Positive	1	1	212696	1	
12	Cpd 12: 2,2,6,6...	2,2,6,6-Tetramethyl-4-pi...	C9 H17 N O	85.65	Pass	826-36-8		155.1316	155.131			6.695	2			Positive	1	1	36289	1	
1	Cpd 1: 10Z-non...	10Z-nonadecenoic acid	C19 H36 O2	84.83	Pass	73033-0...		296.2713	296.2715			9.495	2			Positive	1	1	3365	1	
8	Cpd 8: N-(14-M...	N-(14-Methylhexadecan...	C21 H41 N O	84.06	Pass	260058-...		323.3189	323.3188			17.392	2			Positive	1	1	16790	1	
10	Cpd 10: 1-Tride...	1-Tridecene	C13 H26	83.39	Pass	2437-56...		182.2044	182.2035			9.182	2			Positive	1	1	12764	1	
2	Cpd 2: Pentami...	Pentamidine	C19 H24 N4 O2	74.9	Warning	100-33-4	C07420	340.1883	340.1899			7.369	2			Positive	1	1	2749	1	
19	Cpd 19: Cycloc...	Cyclocalopin D	C23 H32 O13	71.86	Pass			516.1838	516.1843			9.035	4			Positive	2	1	3400	2	
15	Cpd 15: Ribofla...	Riboflavin (Vitamin B2)	C17 H20 N4 O6	65.36	Pass	83-88-5	C00255	376.1411	376.1383			8.818	5			Positive	1	1	13472	1	
9	Cpd 9: Myricato...	Myricatomentoside I	C26 H32 O10	53.16	Pass	191999-...		504.2012	504.1995			7.848	4			Positive	2	1	32197	2	
7	Cpd 7: C21 H4...		C21 H44 N2 O2	49.54	Warning			356.3405		356.3403	-0.52	15.773	3	99.08	-0.19	Positive	1	1	59226	1	
16	Cpd 16: C14 H...		C14 H30 N2 O	49.07	Pass			242.2363		242.2358	-2.09	8.617	3	98.15	-0.51	Positive	1	1	7670	1	
14	Cpd 14: C12 H...		C12 H26 N2 O	48.24	Pass			214.2053		214.2045	-3.51	7.679	3	96.47	-0.75	Positive	1	1	22393	1	
13	Cpd 13: C20 H...		C20 H22 N14...	41.65	Warning			506.2001		506.1999	-0.27	7.853	4	83.31	-0.13	Positive	2	1	22663	2	
11	Cpd 11: C44 H...		C44 H54 N2 O4	40.65	Pass			674.4086		674.4084	-0.31	20.796	8	81.3	-0.21	Positive	1	1	3570	1	
6	Cpd 6: Chlorma...	Chlormadinone acetate	C23 H29 Cl O4	40.22	Pass	302-22-7	C12729	404.1725	404.1754			10.202	4			Positive	1	1	5672	1	
17	Cpd 17: C18 H...		C18 H22 N14...	39.91	Pass			514.1908		514.1898	-2.08	9.034	4	79.81	-1.07	Positive	2	1	3875	2	
5	Cpd 5: Morroni...	Morroniside	C17 H26 O11	39.72	Pass	25406-6...	C17000	406.1409	406.1475			21.149	6			Positive	2	1	3059	2	
18	Cpd 18: C17 H...		C17 H34 N2 O	39.66	Pass			282.2673		282.2671	-0.54	9.603	2	79.33	-0.15	Positive	1	1	4192	1	

Secondary metabolite identification for 19 Entities unic Jmax de 10 à 11

- Best know: 5/19
- Cpd 4: Ethyl menthane carboxamide; C13H25NO @7.732 Score :97.75
- Cpd 12: 2,2,6,6-Tetramethyl-4-piperidinone; C9H17NO @6.695 Score: 85.65
- Cpd 1: 10Z-nonadecenoic acid; C19H36O2 @ 9.495 Score: 84.83
- Cpd 8: N-(14-Methylhexadecanoyl)pyrrolidine; C21H41NO @17.392 Score: 84.06
- Cpd 10: 1-Tridecene; C13 H26 @9.182 Score: 83.39



Secondary metabolite identification for 19 Entities unic Jmax de 10 à 11

- Best know: 5/19
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→*Inhibitors of oleamide hydrolase*

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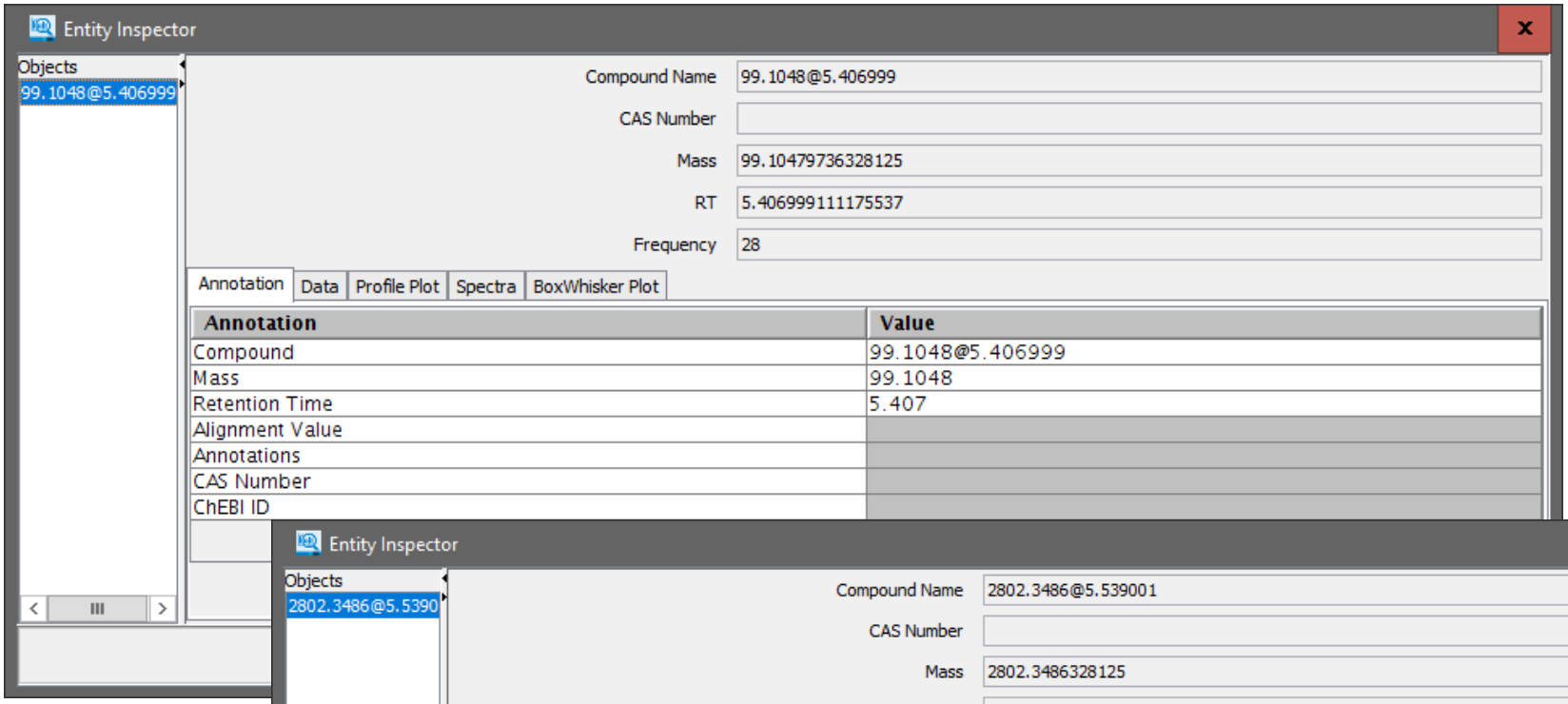
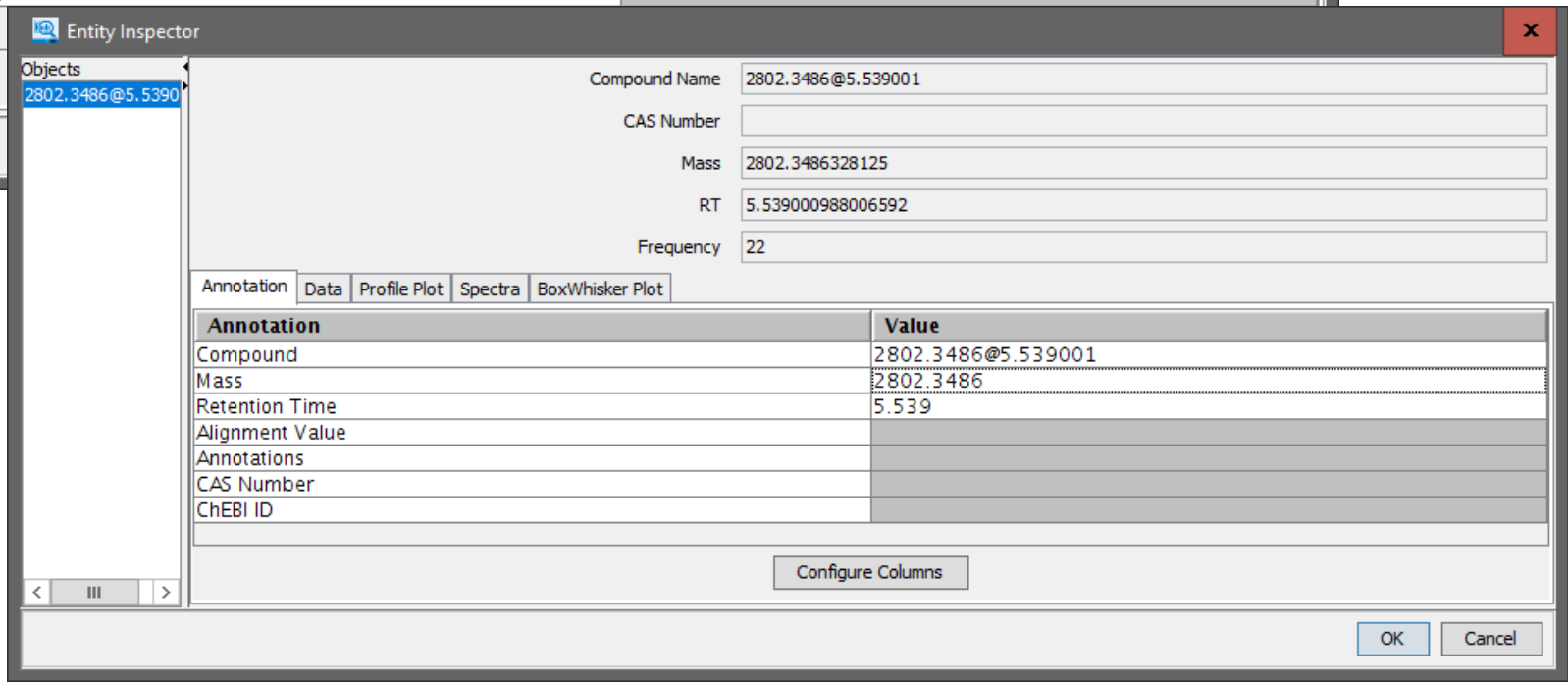
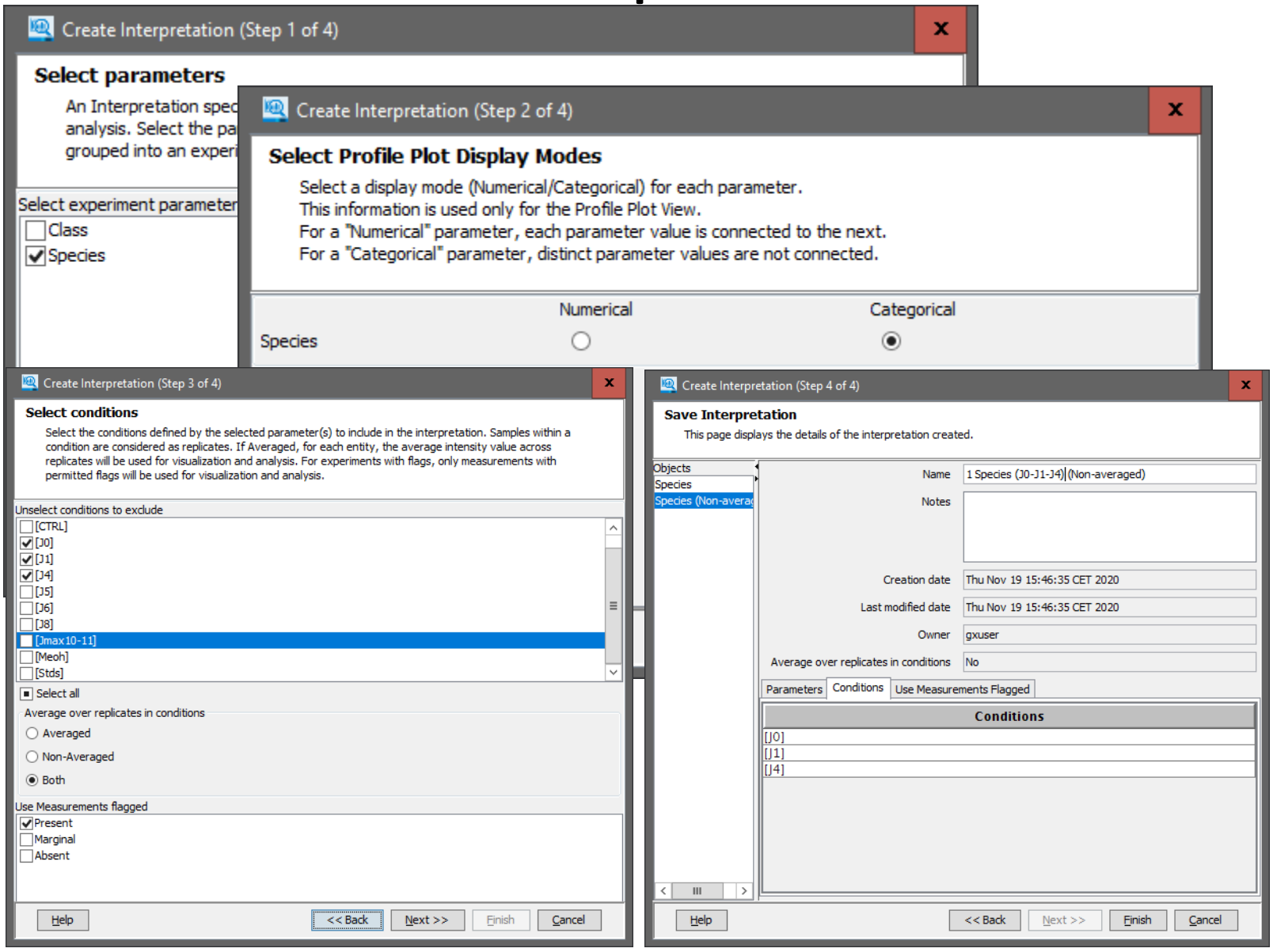
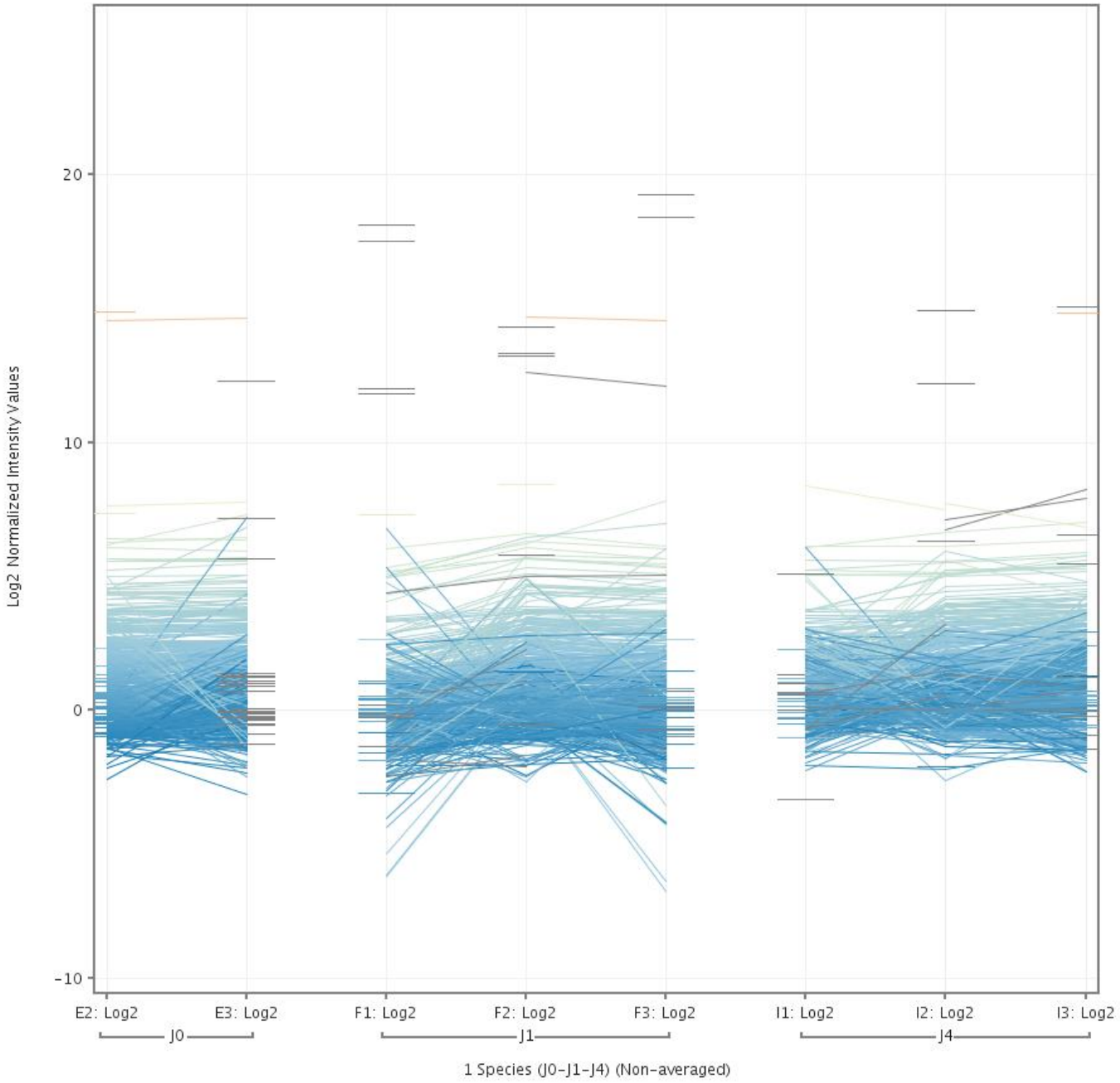
SUITE
avec pour info pour Benoit :
le plus petit métabolite analysé et le plus grand.

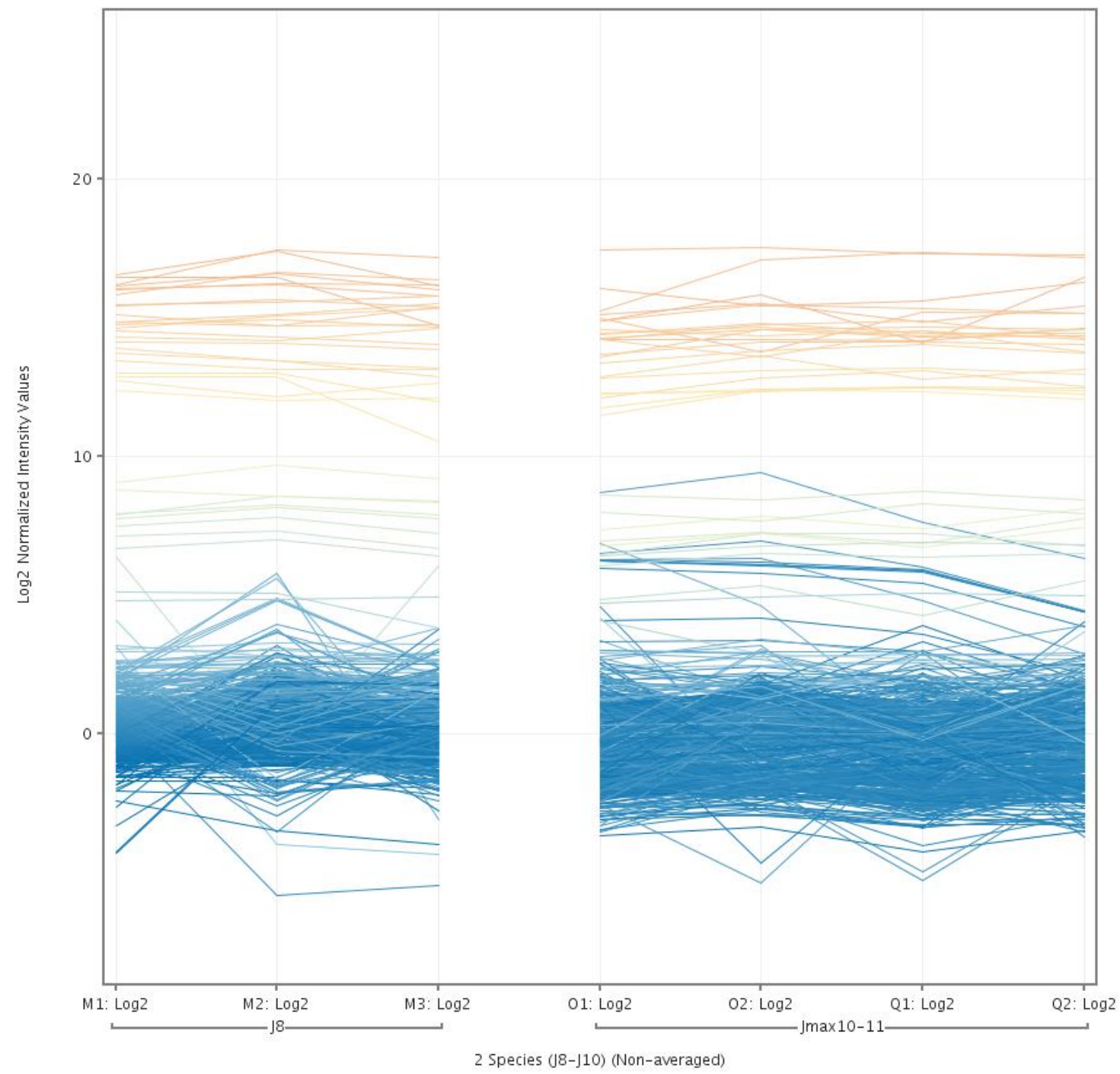


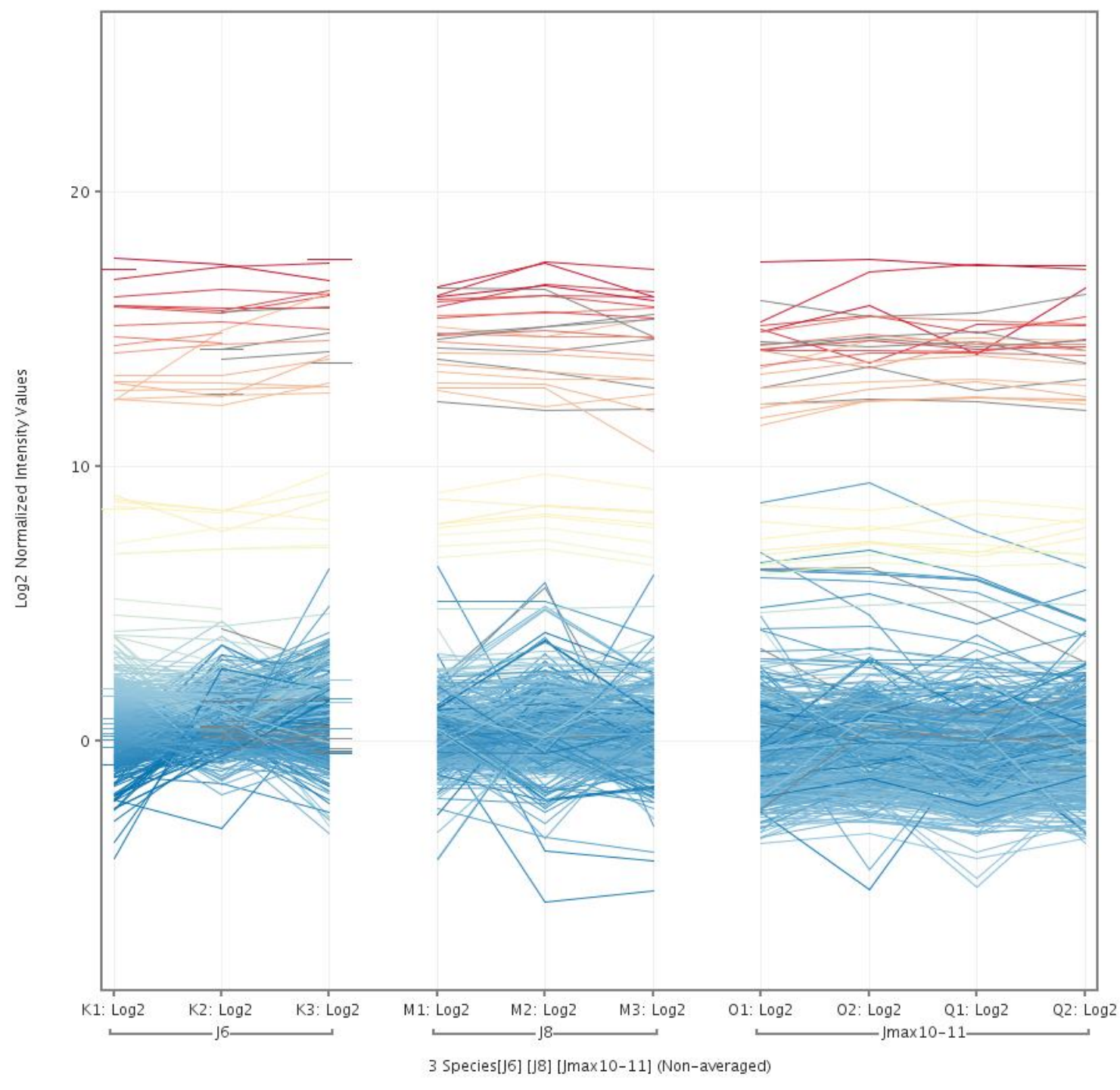


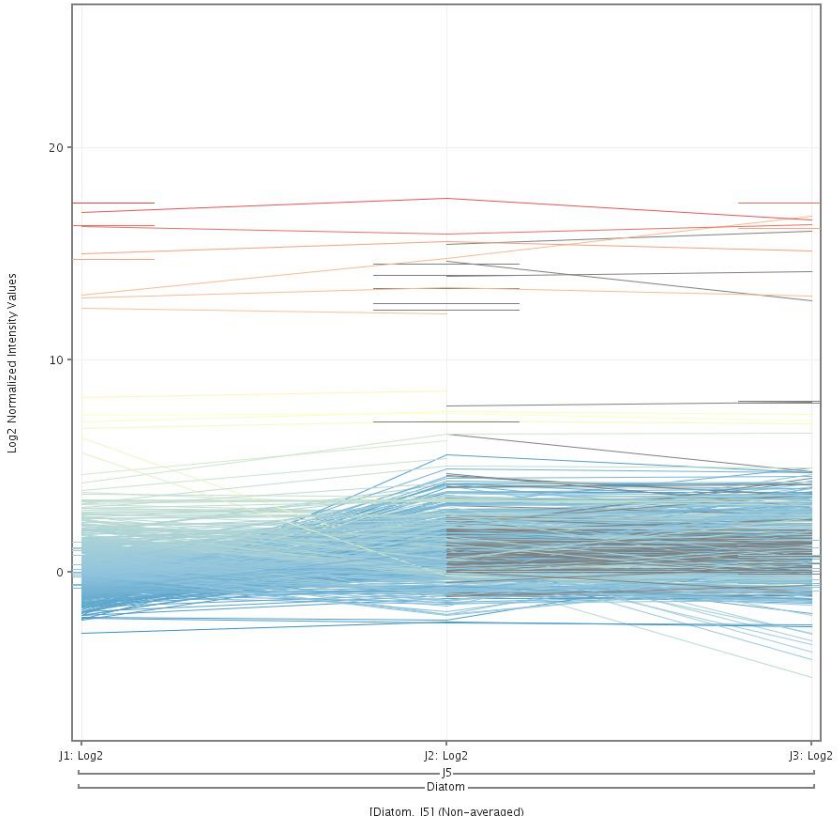
Créations des nouvelles interprétations

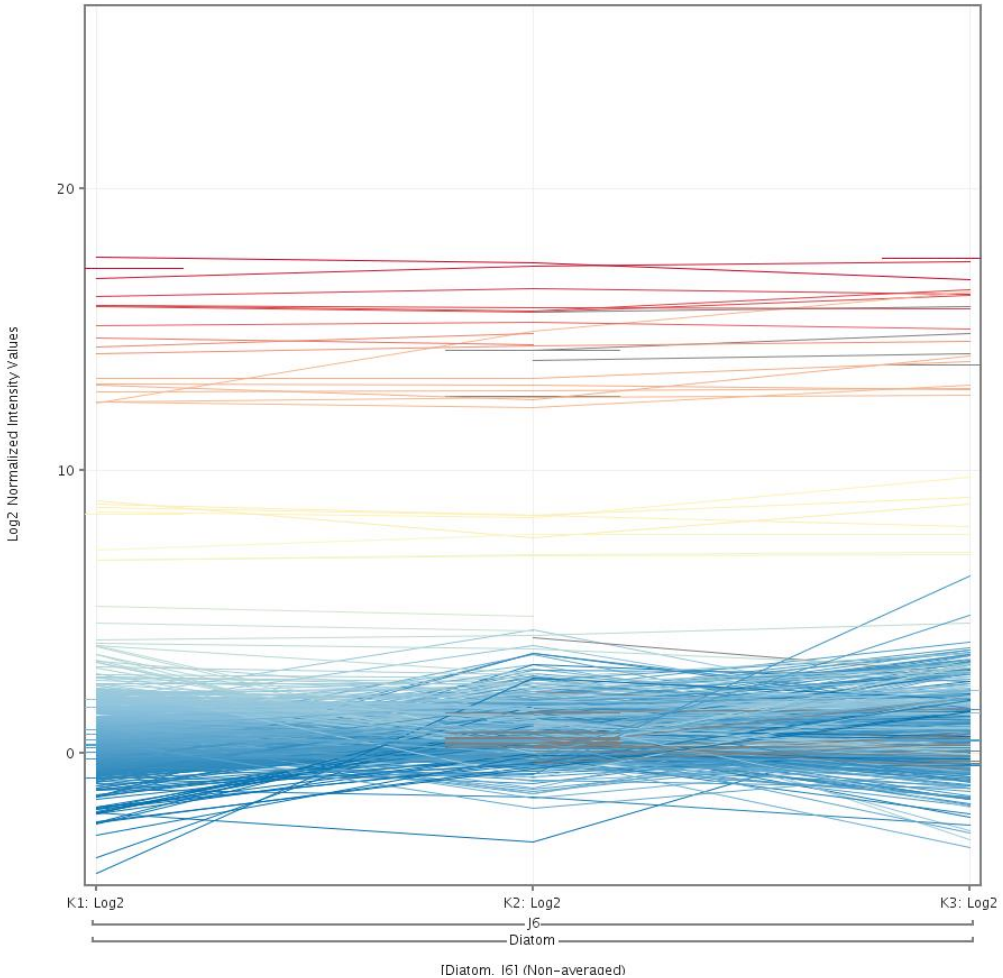


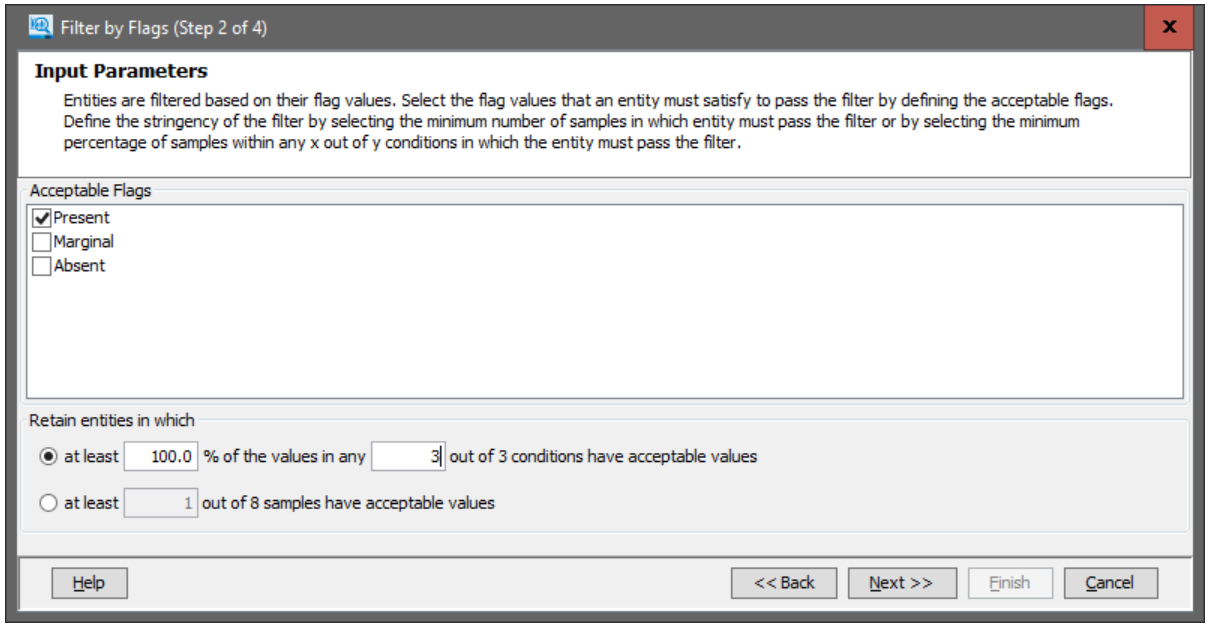

Log2 Normalized Intensity Values
20
10
0
-10
E2: Log2
E3: Log2
F1: Log2
F2: Log2
F3: Log2
I1: Log2
I2: Log2
I3: Log2
J0
J1
J4
1 Species (J0-J1-J4) (Non-averaged)


20
10
0
Log2 Normalized Intensity Values
M1: Log2
M2: Log2
M3: Log2
O1: Log2
O2: Log2
Q1: Log2
Q2: Log2
J8
Jmax10-11
2 Species (J8-J10) (Non-averaged)


Log2 Normalized Intensity Values
20
10
0
K1: Log2
K2: Log2
K3: Log2
M1: Log2
M2: Log2
M3: Log2
O1: Log2
O2: Log2
Q1: Log2
Q2: Log2
J6
J8
Jmax10-11
3 Species[J6] [J8] [Jmax10-11] (Non-averaged)


Log2 Normalized Intensity Values
20
10
0
J1: Log2
J2: Log2
J3: Log2
J5
Diatom
[Diatom, J51 (Non-averaged)


Log2 Normalized Intensity Values
20
10
0
K1: Log2
K2: Log2
K3: Log2
J6
Diatom
[Diatom, J61 (Non-averaged)



Création de l'analyse I correspondante

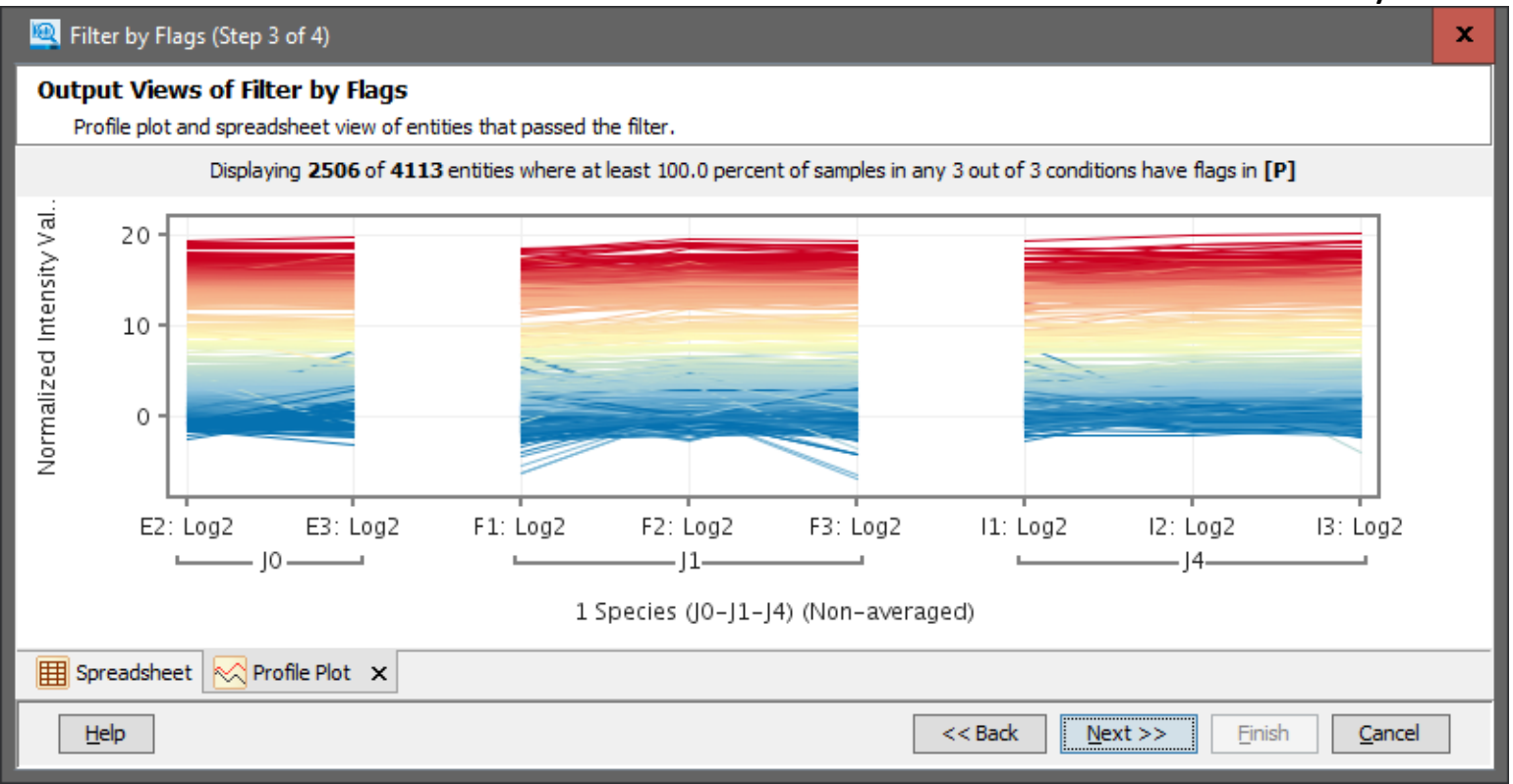
Hy1= J0+JJ+J4

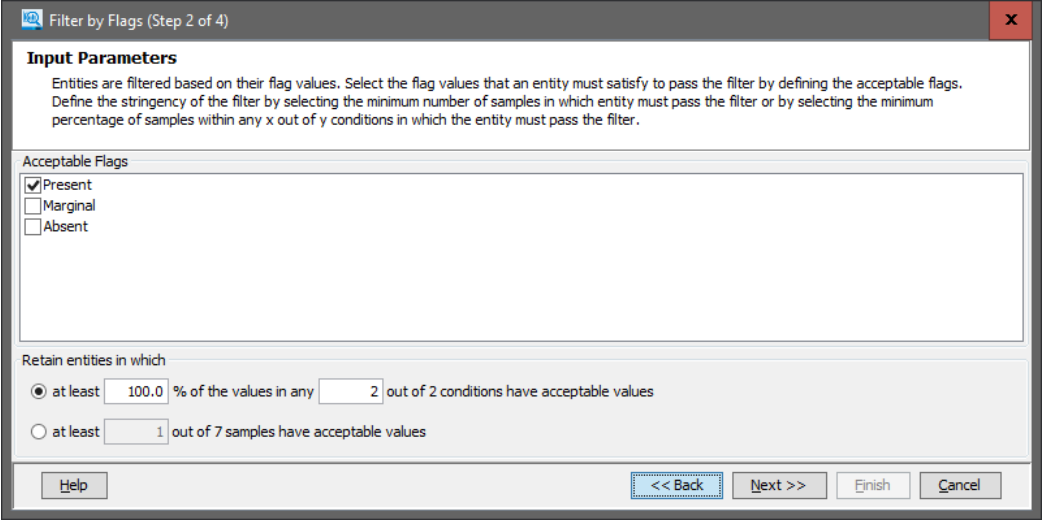
- J5
- J6

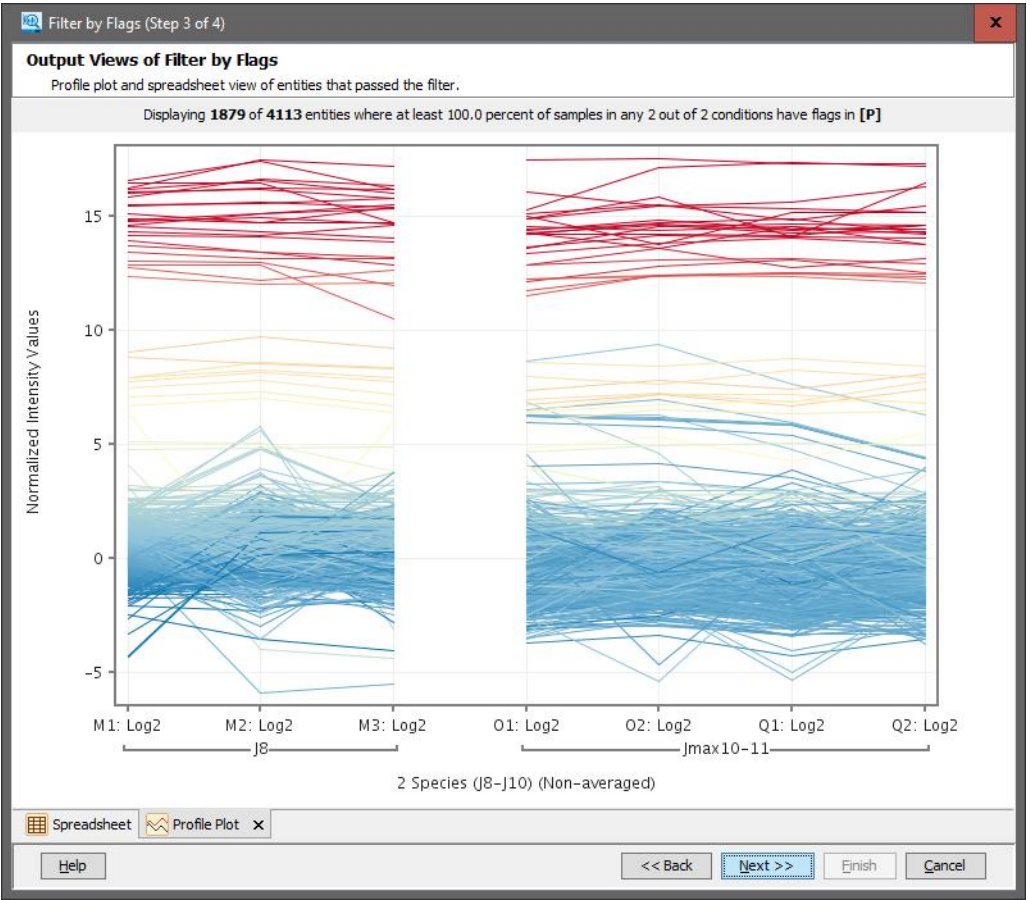
Hy2= J8+Jmax

Avec hy1 100% of the values in any 3 out of 3 conditions have acceptable values

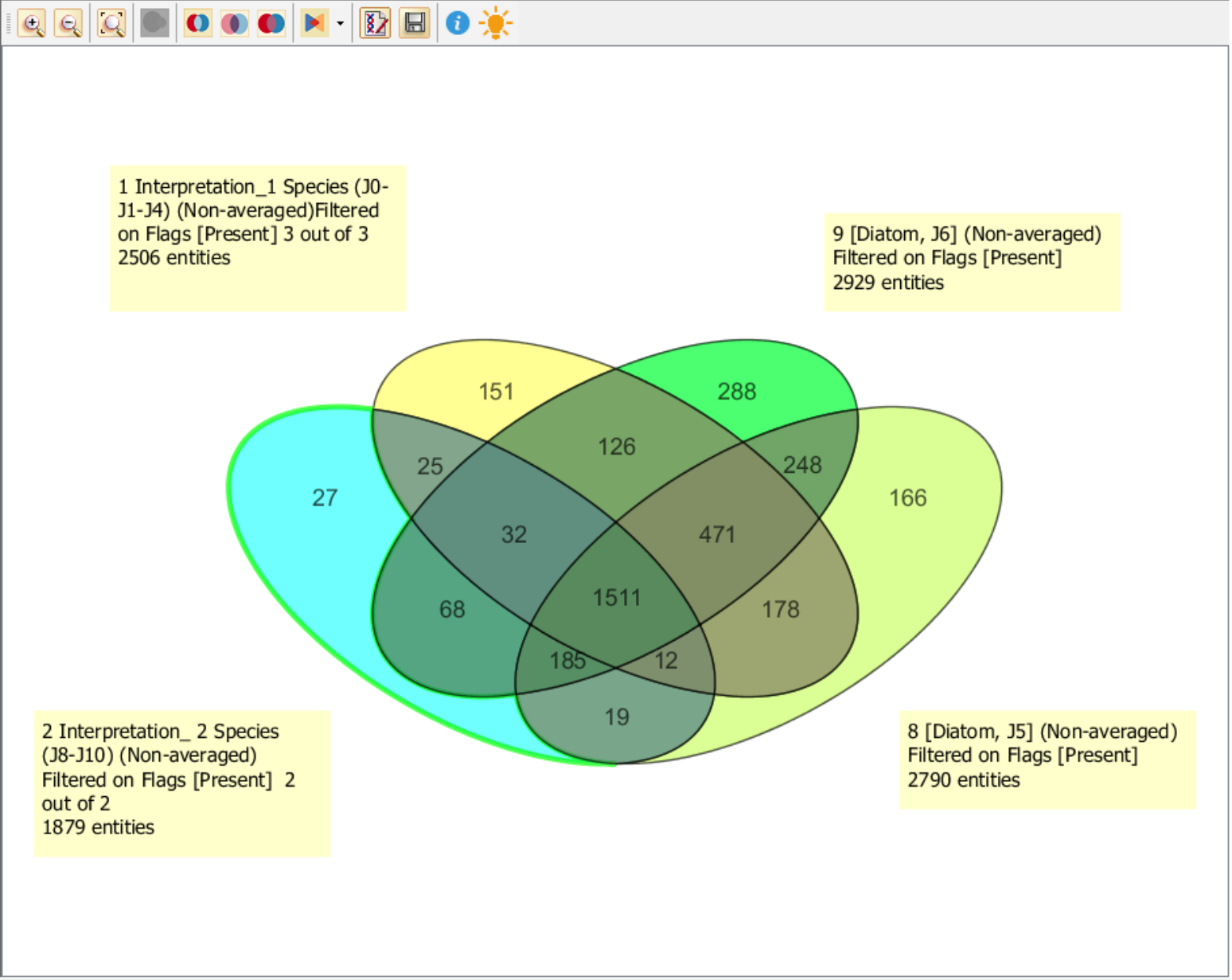
Et Hy2 2 out of 2





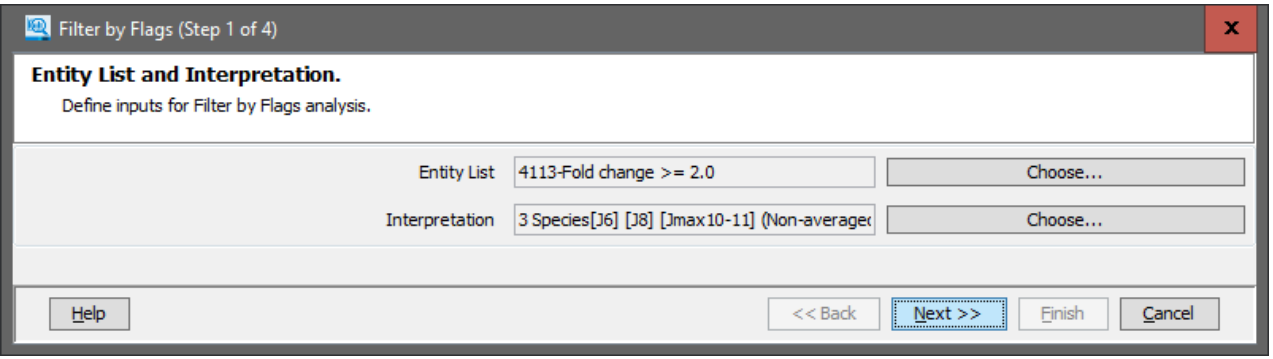


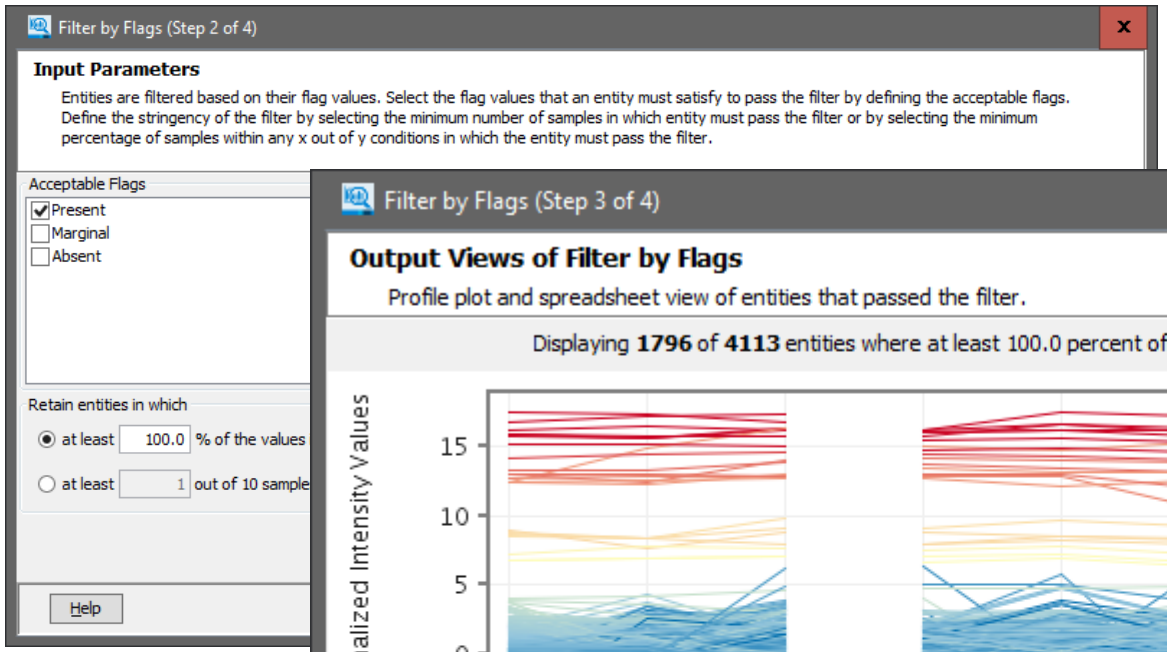
Et Hy2 2 out of 2



Venn Summary | Entity Match Inspector

Color	Experiment Name	Entity List	Count in Experiment	Count in Venn
	Phaeodactylum tricornutum-2020	1 Interpretation_1 Species (J0-J1-J4) (Non-averaged)Filtered on Flags [Present] 3 out of 3	2506	2506
	Phaeodactylum tricornutum-2020	2 Interpretation_ 2 Species (J8-J10) (Non-averaged)Filtered on Flags [Present] 2 out of 2	1879	1879
	Phaeodactylum tricornutum-2020	8 [Diatom, J5] (Non-averaged)Filtered on Flags [Present]	2790	2790
	Phaeodactylum tricornutum-2020	9 [Diatom, J6] (Non-averaged)Filtered on Flags [Present]	2929	2929



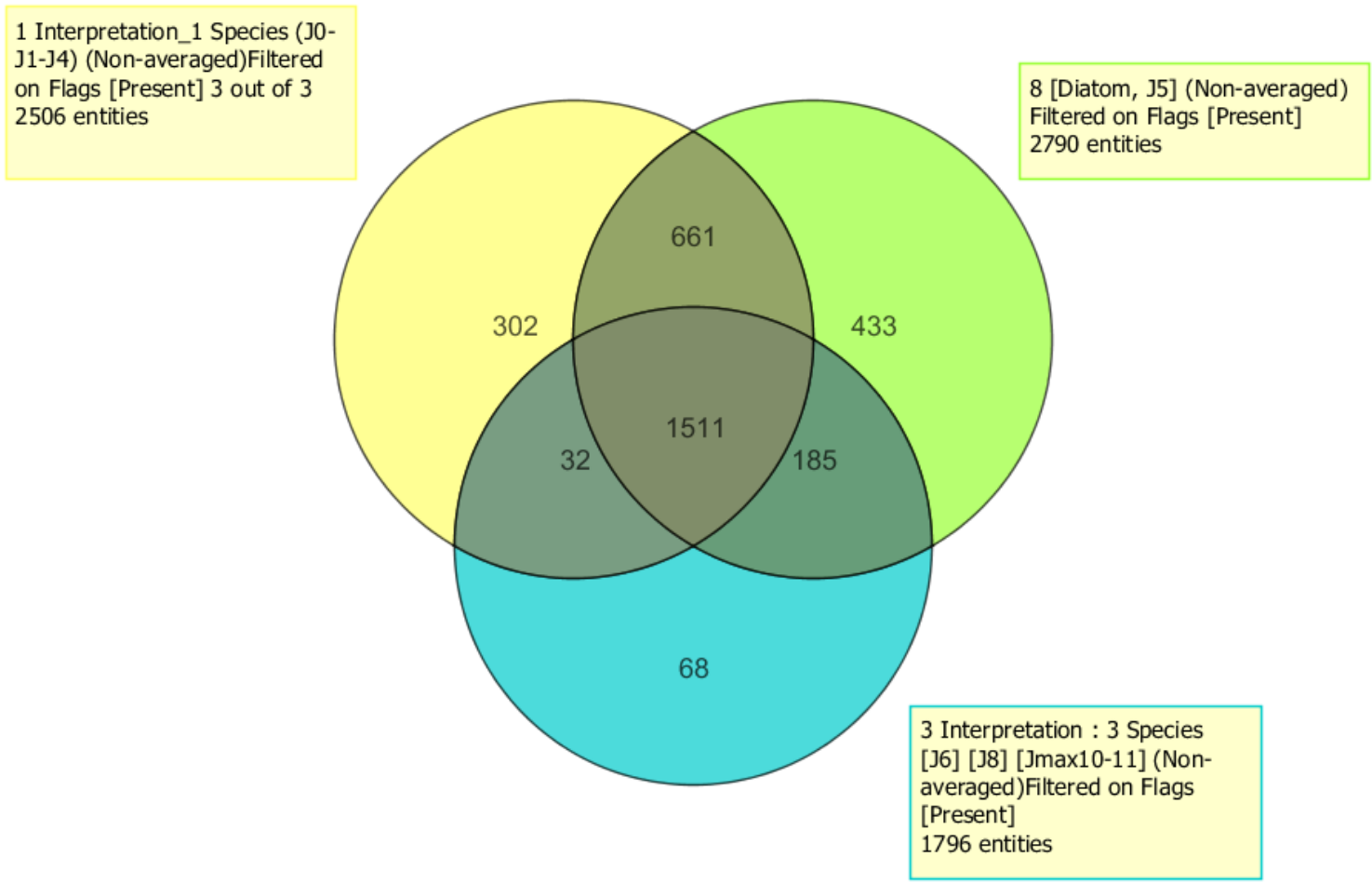


Création de l'analyse II

Hy1= J0+JJ+J4

- J5
- Hy3=J6+ J8+Jmax

Avec hy1 et 3 100% of the values in any 3 out of 3 conditions have acceptable values



Venn Summary | Entity Match Inspector

Color	Experiment Name	Entity List	Count in Experiment	Count in Venn
☑	Phaeodactylum tricornutum-2020	1 Interpretation_1 Species (J0-J1-J4) (Non-averaged)Filtered on Flags [Present] 3 out of 3	2506	2506
☑	Phaeodactylum tricornutum-2020	8 [Diatom, J5] (Non-averaged)Filtered on Flags [Present]	2790	2790
☑	Phaeodactylum tricornutum-2020	3 Interpretation : 3 Species[J6] [J8] [Jmax10-11] (Non-averaged)Filtered on Flags [Present]	1796	1796

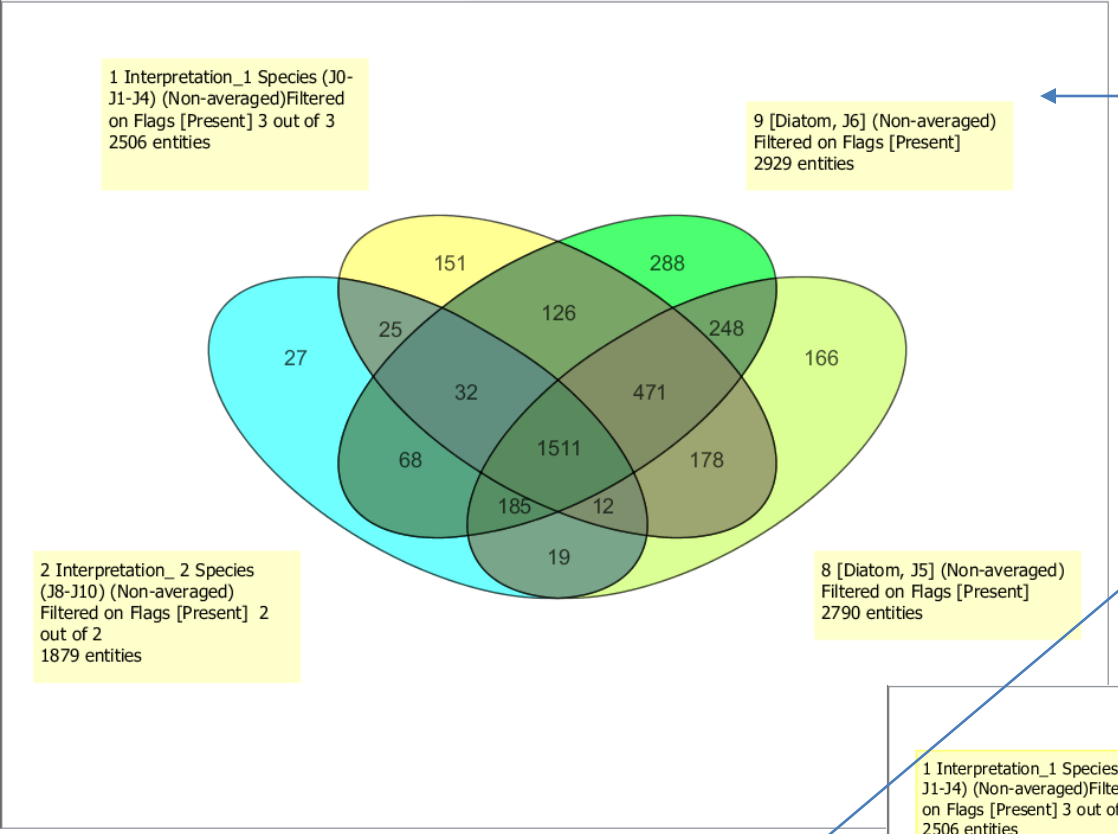
Comparaison

Analyse 1:

Hy1= J0+JJ+J4
- J5
- J6

Hy2= J8+Jmax

Avec hy1 100% of the values in any 3 out of 3 conditions have acceptable values
Et Hy2 2 out of 2



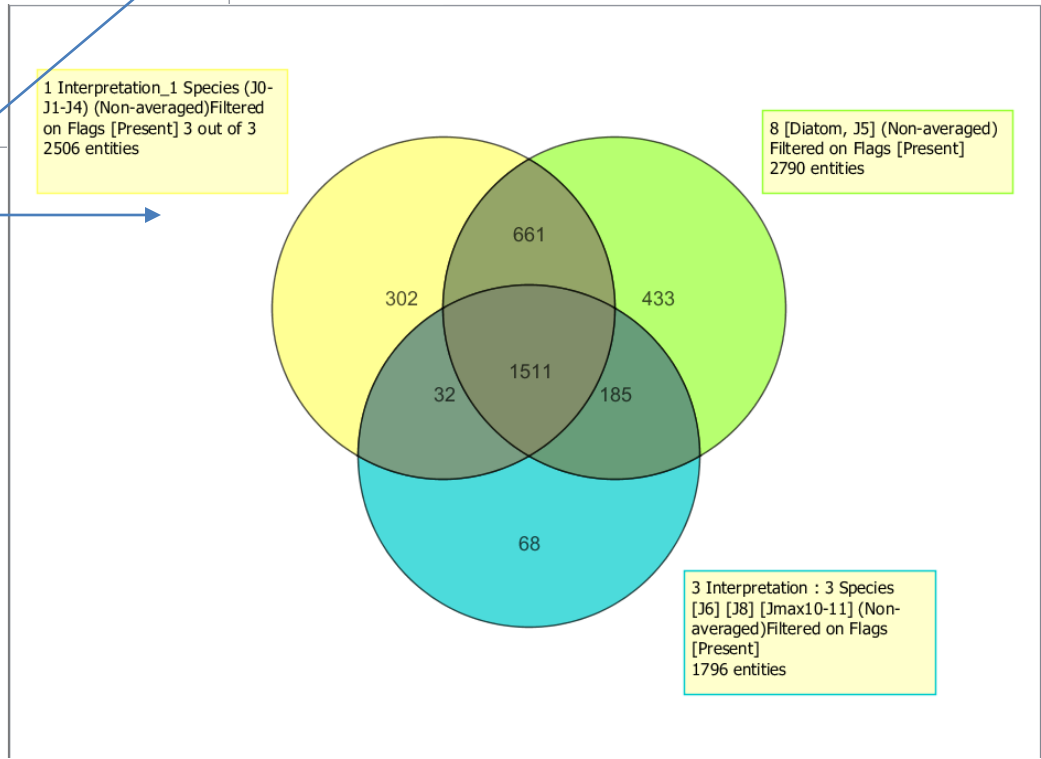
VS

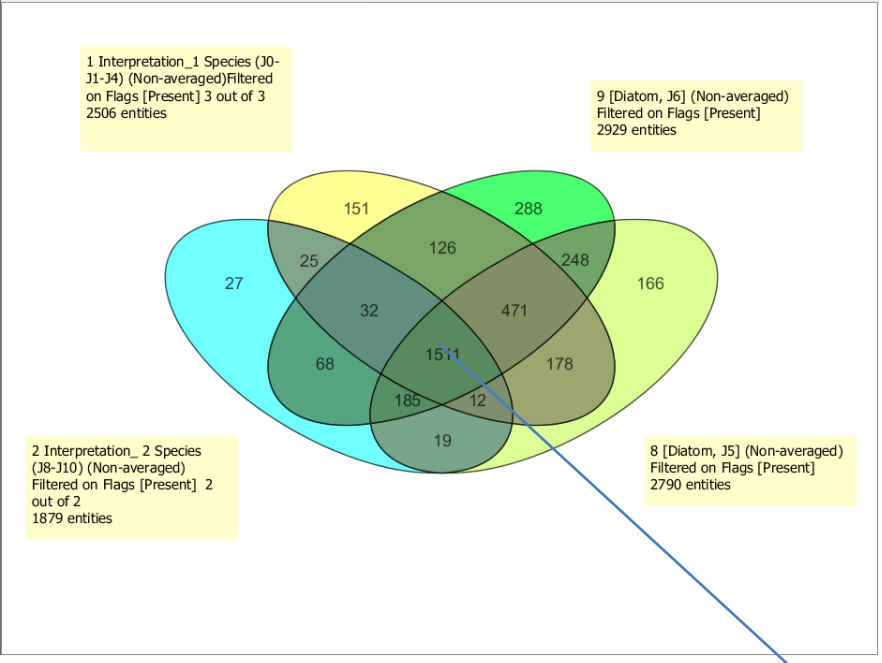
Analyse II:

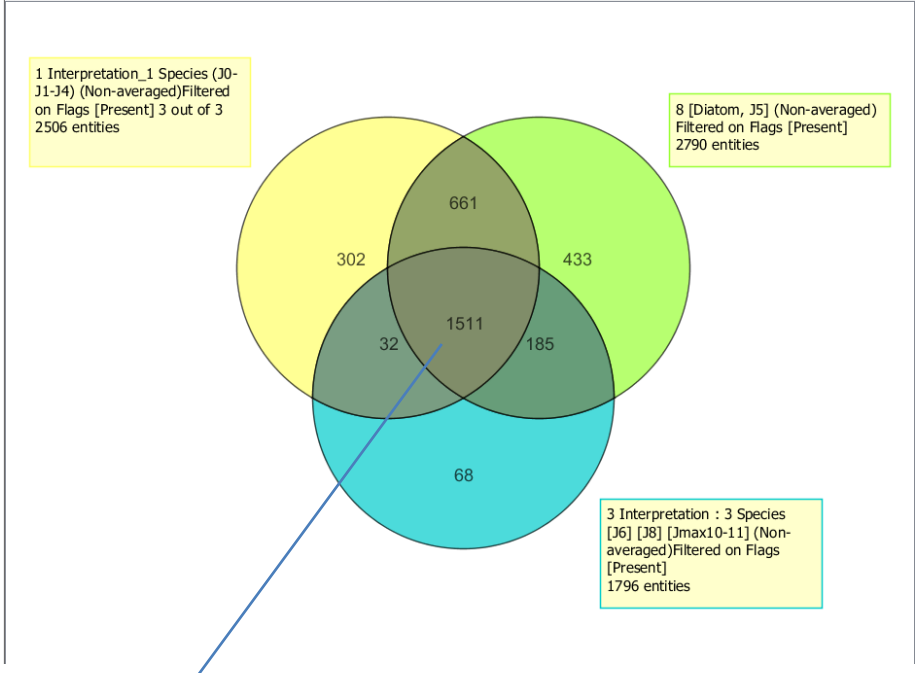
Hy1= J0+JJ+J4
- J5
- Hy3=J6+ J8+Jmax

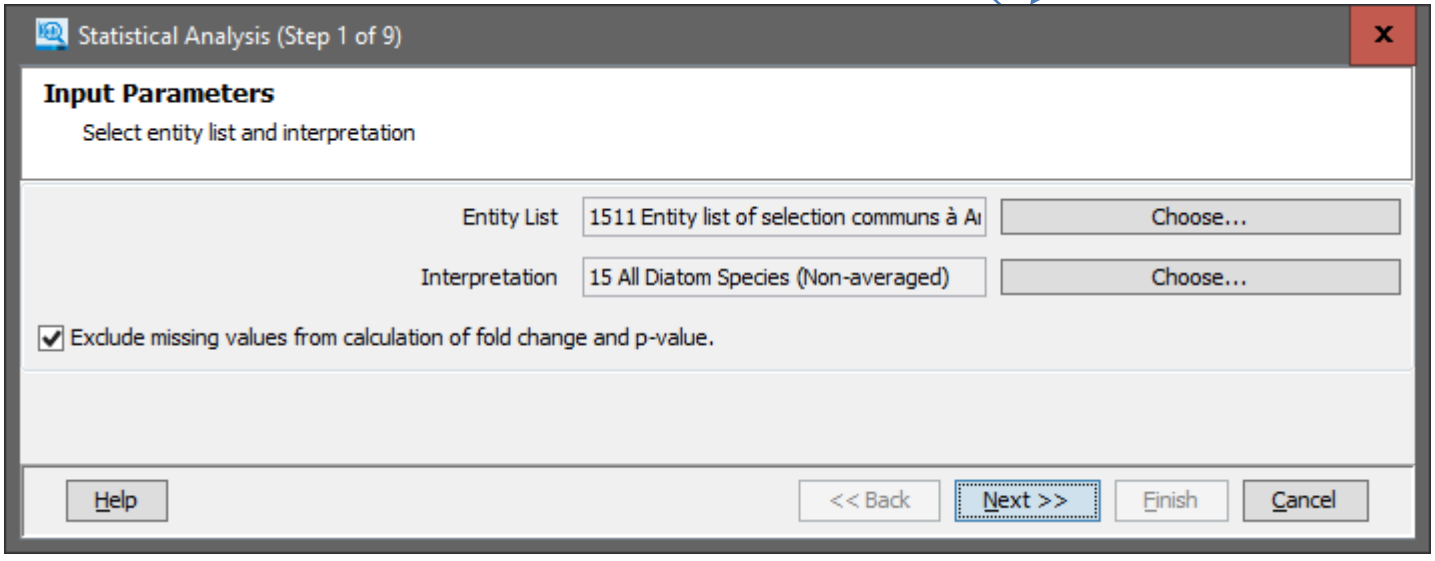
Avec hy1 et Hy3

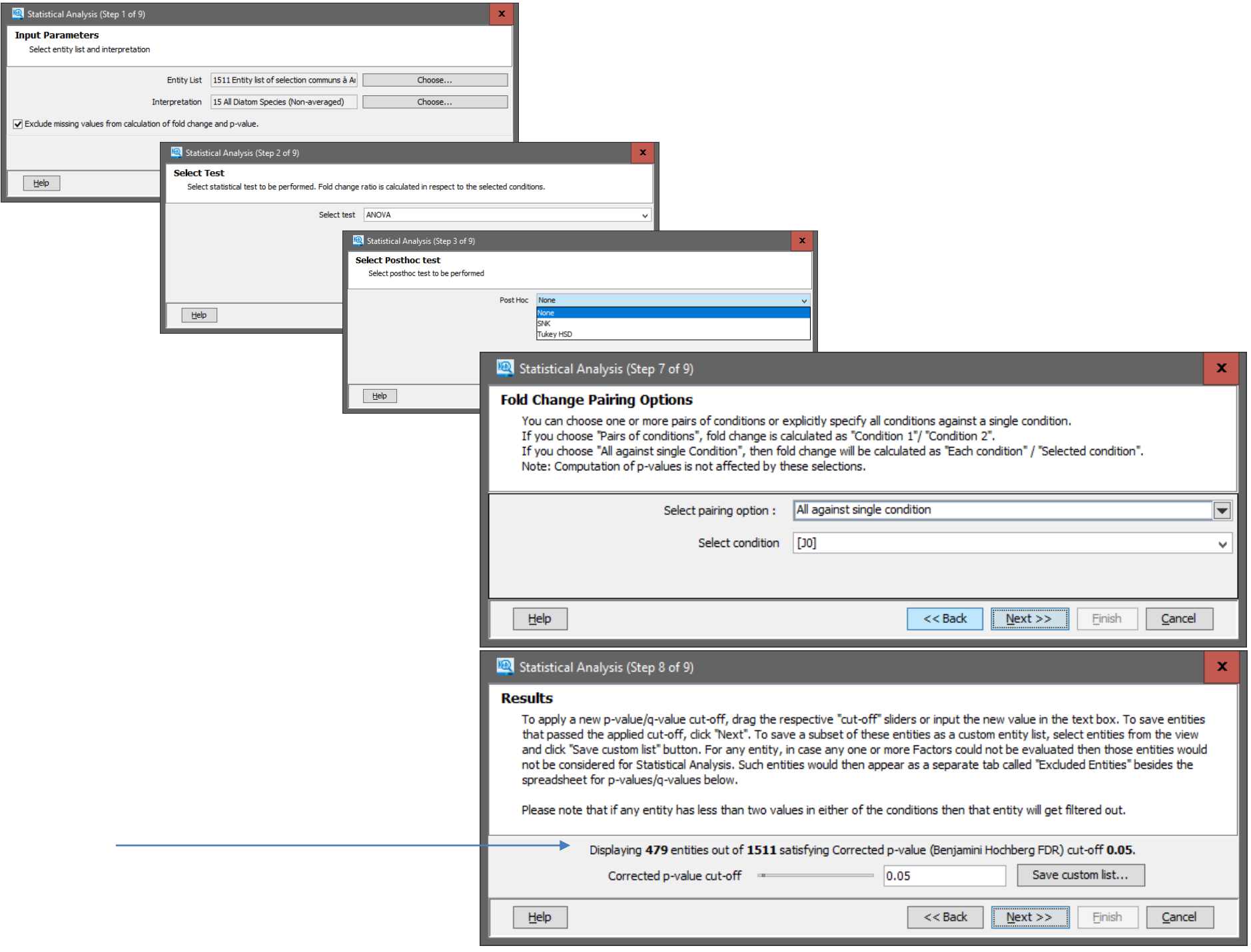
100% of the values in any 3 out of 3 conditions have acceptable values

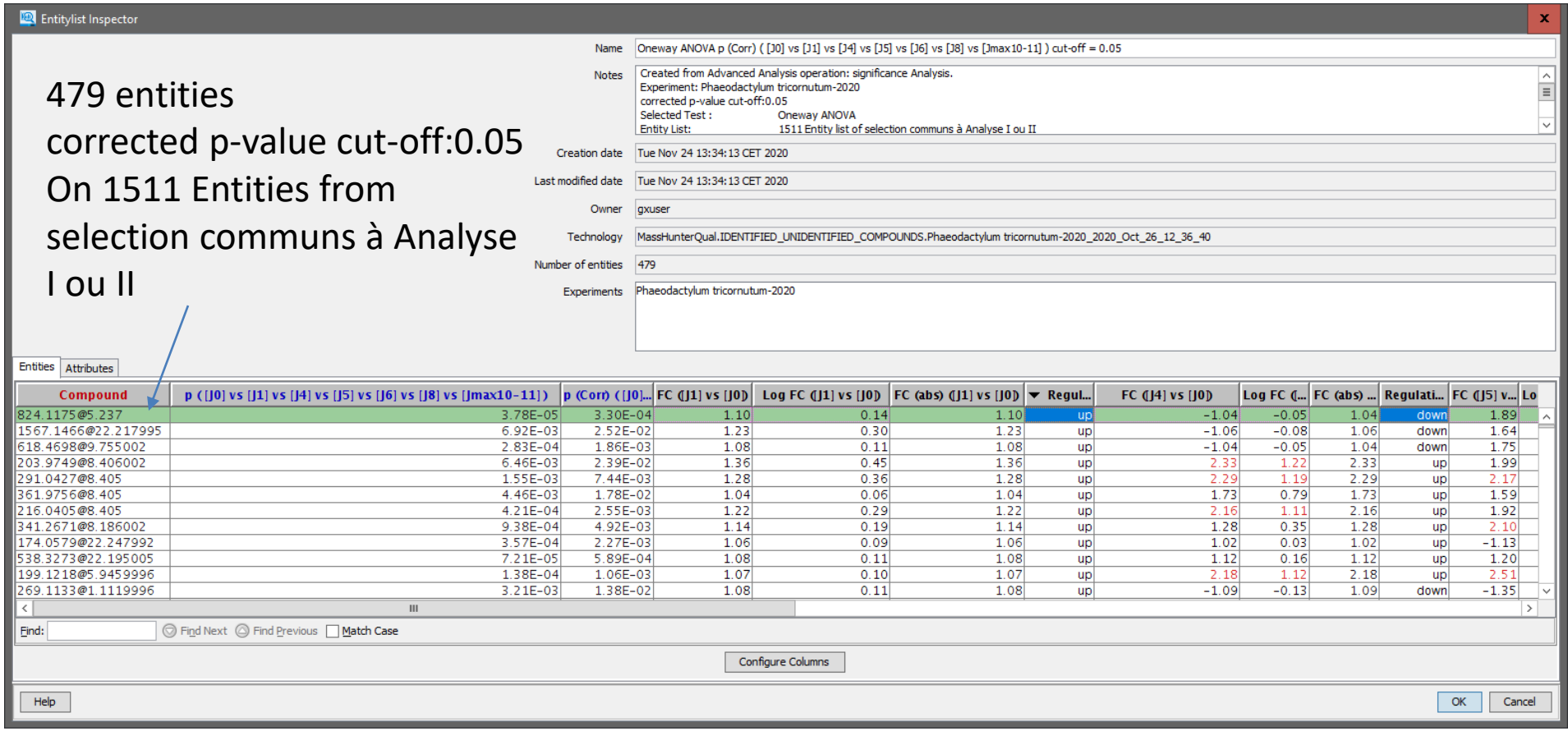



1 Interpretation_1 Species (J0-J1-J4) (Non-averaged)Filtered on Flags [Present] 3 out of 3
2506 entities
9 [Diatom, J6] (Non-averaged) Filtered on Flags [Present]
2929 entities
151
288
126
25
248
27
166
32
471
68
1511
178
185
12
19
2 Interpretation_ 2 Species (J8-J10) (Non-averaged) Filtered on Flags [Present] 2 out of 2
1879 entities
8 [Diatom, J5] (Non-averaged) Filtered on Flags [Present]
2790 entities


1 Interpretation_1 Species (J0-J1-J4) (Non-averaged)Filtered on Flags [Present] 3 out of 3
2506 entities
8 [Diatom, J5] (Non-averaged) Filtered on Flags [Present]
2790 entities
661
302
433
1511
32
185
68
3 Interpretation : 3 Species [J6] [J8] [Jmax10-11] (Non-averaged)Filtered on Flags [Present]
1796 entities

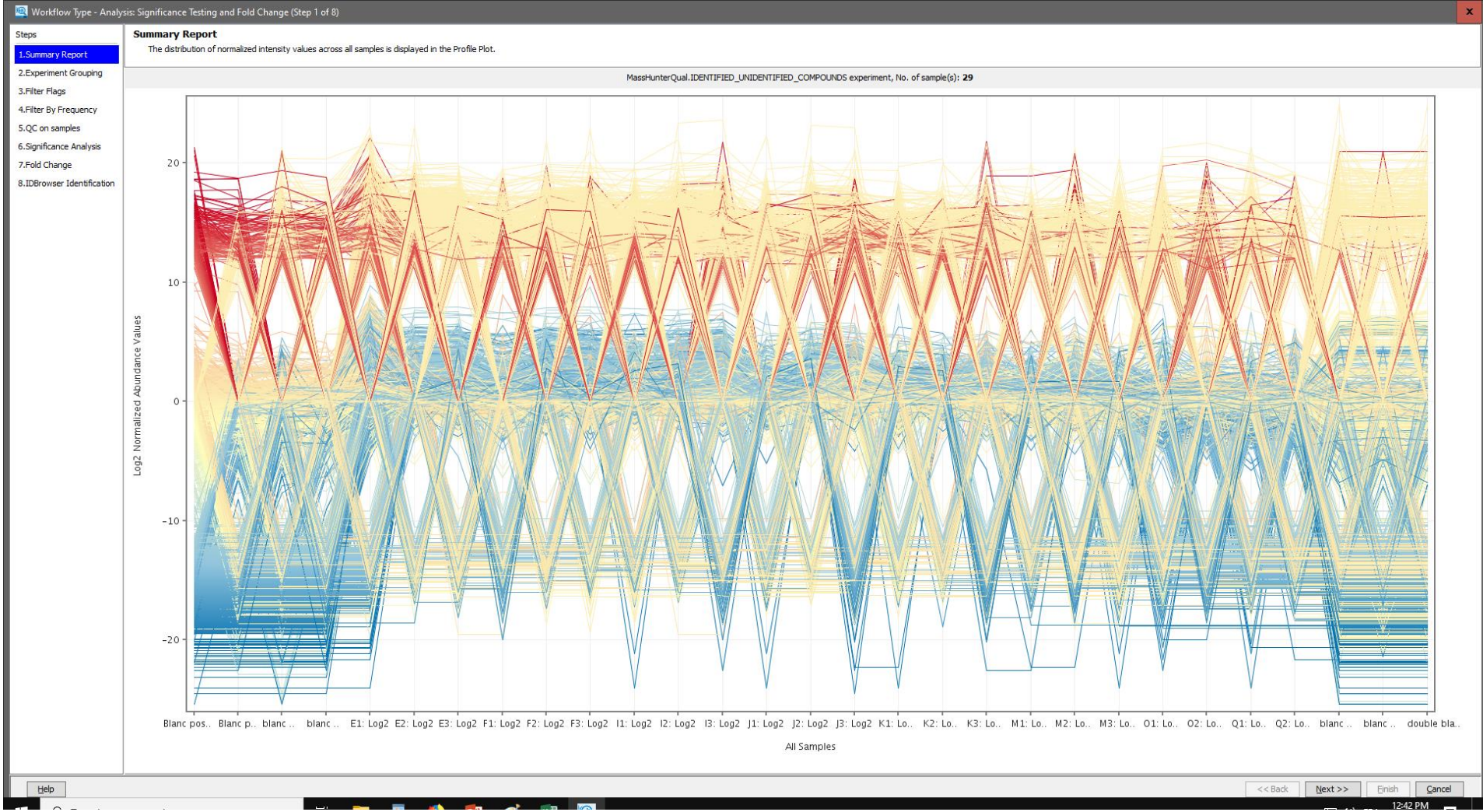

Statistical Analysis (Step 1 of 9)
Input Parameters
Select entity list and interpretation
Entity List
1511 Entity list of selection communs à Ai
Choose...
Interpretation
15 All Diatom Species (Non-averaged)
Choose...
Exclude missing values from calculation of fold change and p-value.
Help
<< Back
Next >>
Finish
Cancel


Statistical Analysis (Step 1 of 9)
Input Parameters
Select entity list and interpretation
Entity List
1511 Entity list of selection communs à Ai
Choose...
Interpretation
15 All Diatom Species (Non-averaged)
Choose...
Exclude missing values from calculation of fold change and p-value.
Help
Statistical Analysis (Step 2 of 9)
Select Test
Select statistical test to be performed. Fold change ratio is calculated in respect to the selected conditions.
Select test
ANOVA
Help
Statistical Analysis (Step 3 of 9)
Select Posthoc test
Select posthoc test to be performed
Post Hoc
None
None
SNK
Tukey HSD
Help
Statistical Analysis (Step 7 of 9)
Fold Change Pairing Options
You can choose one or more pairs of conditions or explicitly specify all conditions against a single condition.
If you choose "Pairs of conditions", fold change is calculated as "Condition 1"/ "Condition 2".
If you choose "All against single Condition", then fold change will be calculated as "Each condition" / "Selected condition".
Note: Computation of p-values is not affected by these selections.
Select pairing option :
All against single condition
Select condition
[J0]
Help
<< Back
Next >>
Finish
Cancel
Statistical Analysis (Step 8 of 9)
Results
To apply a new p-value/q-value cut-off, drag the respective "cut-off" sliders or input the new value in the text box. To save entities that passed the applied cut-off, click "Next". To save a subset of these entities as a custom entity list, select entities from the view and click "Save custom list" button. For any entity, in case any one or more Factors could not be evaluated then those entities would not be considered for Statistical Analysis. Such entities would then appear as a separate tab called "Excluded Entities" besides the spreadsheet for p-values/q-values below.
Please note that if any entity has less than two values in either of the conditions then that entity will get filtered out.
Displaying 479 entities out of 1511 satisfying Corrected p-value (Benjamini Hochberg FDR) cut-off 0.05.
Corrected p-value cut-off
0.05
Save custom list...
Help
<< Back
Next >>
Finish
Cancel

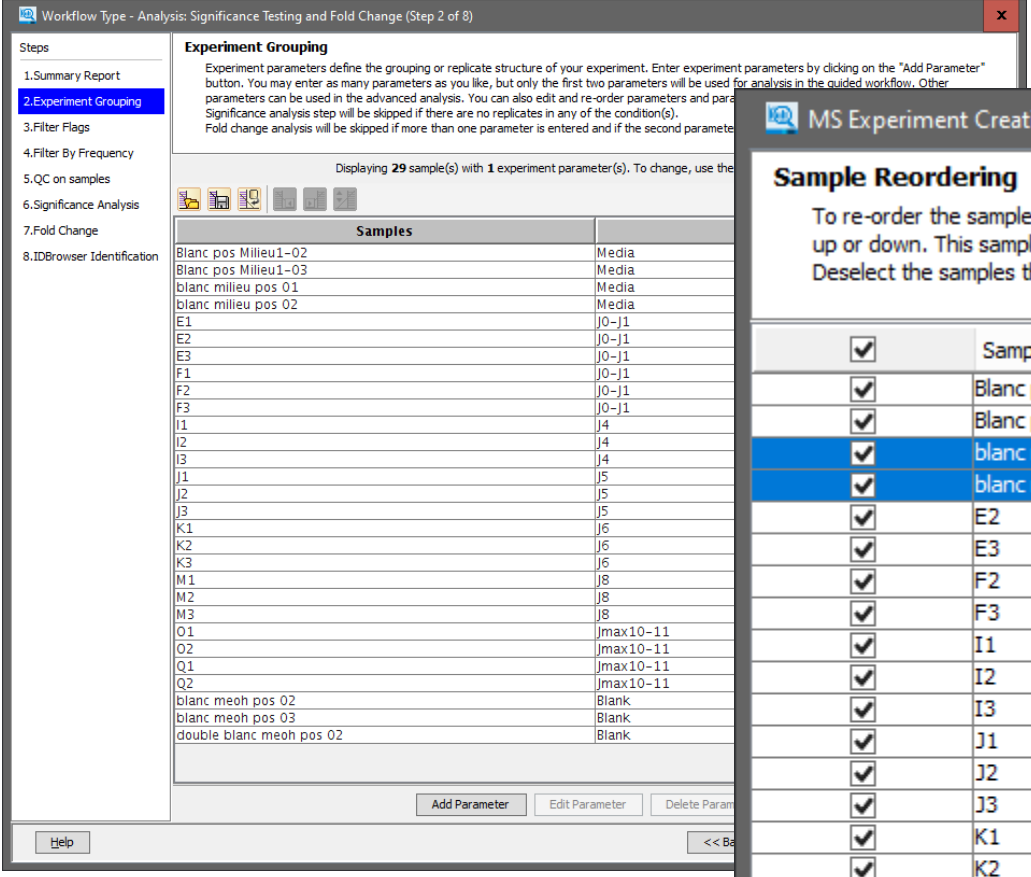


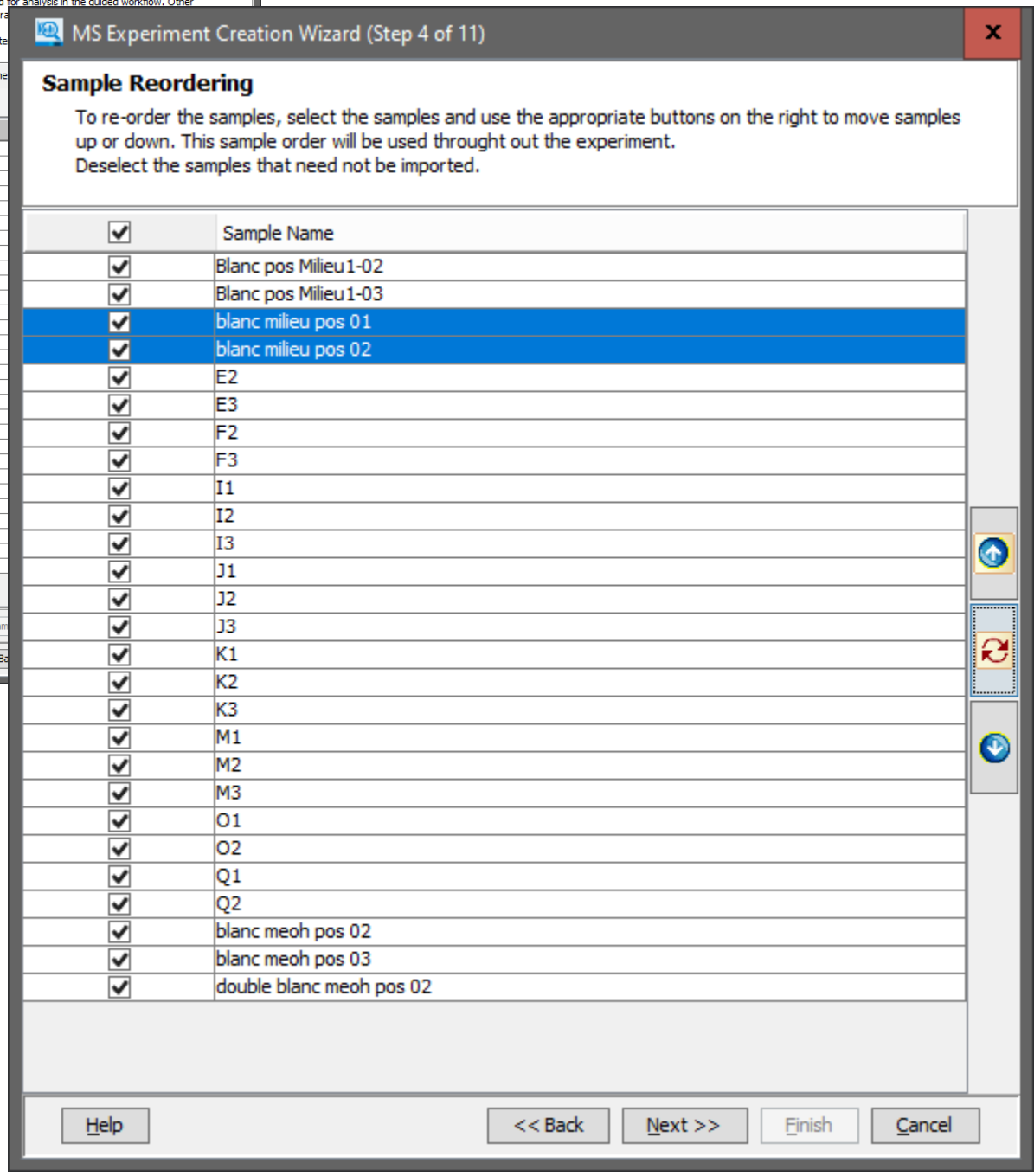
Created from Advanced Analysis operation: significance Analysis.
Experiment: Phaeodactylum tricornutum-2020
corrected p-value cut-off:0.05
Selected Test : Oneway ANOVA
Entity List: 1511 Entity list of selection communs à Analyse I ou II
Interpretation: 15 All Diatom Species (Non-averaged)
p-value computation: Asymptotic
Multiple Testing Correction: Benjamini-Hochberg

SUITE II



Nouvel « experiment » basé sur 27 échantillons seulement Phaeodactylum (without E1 et F1)+ Media + Solvant


Workflow Type - Analysis: Significance Testing and Fold Change (Step 2 of 8)
Steps
1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification
Experiment Grouping
Experiment parameters define the grouping or replicate structure of your experiment. Enter experiment parameters by clicking on the "Add Parameter" button. You may enter as many parameters as you like, but only the first two parameters will be used for analysis in the guided workflow. Other parameters can be used in the advanced analysis. You can also edit and re-order parameters and para
Significance analysis step will be skipped if there are no replicates in any of the condition(s).
Fold change analysis will be skipped if more than one parameter is entered and if the second paramete
Displaying 29 sample(s) with 1 experiment parameter(s). To change, use the
Samples
Blanc pos Milieu1-02 Media
Blanc pos Milieu1-03 Media
blanc milieu pos 01 Media
blanc milieu pos 02 Media
E1 J0-J1
E2 J0-J1
E3 J0-J1
F1 J0-J1
F2 J0-J1
F3 J0-J1
I1 J4
I2 J4
I3 J4
J1 J5
J2 J5
J3 J5
K1 J6
K2 J6
K3 J6
M1 J8
M2 J8
M3 J8
O1 Jmax10-11
O2 Jmax10-11
Q1 Jmax10-11
Q2 Jmax10-11
blanc meoh pos 02 Blank
blanc meoh pos 03 Blank
double blanc meoh pos 02 Blank
Add Parameter
Edit Parameter
Delete Param
Help
<< Ba


MS Experiment Creation Wizard (Step 4 of 11)
Sample Reordering
To re-order the samples, select the samples and use the appropriate buttons on the right to move samples up or down. This sample order will be used throught out the experiment.
Deselect the samples that need not be imported.
Sample Name
Blanc pos Milieu1-02
Blanc pos Milieu1-03
blanc milieu pos 01
blanc milieu pos 02
E2
E3
F2
F3
I1
I2
I3
J1
J2
J3
K1
K2
K3
M1
M2
M3
O1
O2
Q1
Q2
blanc meoh pos 02
blanc meoh pos 03
double blanc meoh pos 02
Help
<< Back
Next >>
Finish
Cancel

MS Experiment Creation Wizard (Step 9 of 11)

Sample Summary

From the Entities tab, use merging options to manually merge entities. Spectra of selected entities are displayed to help merging.
Compound Frequency tab displays the frequency of aligned compounds across all the samples.
Mass vs RT tab displays a scatter plot of compounds and spreadsheet has the summary of aligned compounds present or absent in individual samples.

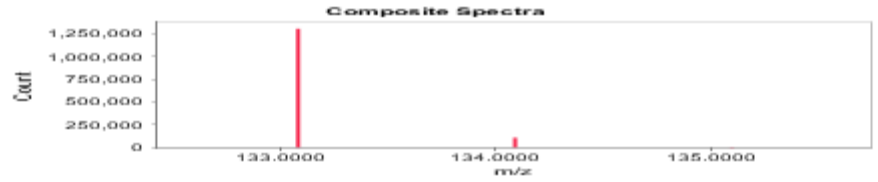
Export For Recursion

Total number of Aligned Compounds = **6263**

Entities | Compound Frequency | Mass vs RT

Merged	Compound	Mass	Retention Time
	132.069@6.07...	132.0690	6.072
	658.4239@20....	658.4239	20.819
	829.5867@20....	829.5867	20.883
	610.1612@22....	610.1612	22.718
	790.4642@22....	790.4642	22.251
	390.2778@23....	390.2778	23.309
	180.095@7.26...	180.0950	7.266
	337.1753@3.6...	337.1753	3.643
	325.3714@17....	325.3714	17.400
	785.5088@22....	785.5088	22.243
	792.4799@23....	792.4799	23.026
	558.1244@21....	558.1244	21.358
	658.4241@20....	658.4241	20.819
	370.0943@21....	370.0943	21.366
	803.5699@20....	803.5699	20.553

Preview Merged Entity Spectra



Help | << Back | Next >> | Finish | Cancel

MS Experiment Creation Wizard (Step 9 of 11)

Sample Summary

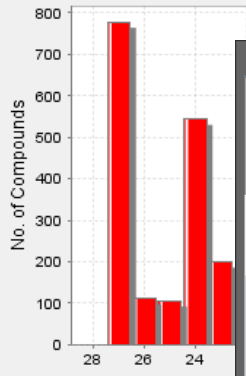
From the Entities tab, use merging options to manually merge entities. Spectra of selected entities are displayed to help merging.
Compound Frequency tab displays the frequency of aligned compounds across all the samples.
Mass vs RT tab displays a scatter plot of compounds and spreadsheet has the summary of aligned compounds present or absent in individual samples.

Export For Recursion

Total number of Aligned Compounds = **6263**

Entities | Compound Frequency | Mass vs RT

Total Samples: 27



Frequency	Number
27	778
26	111
25	106
24	544

Help

MS Experiment Creation Wizard (Step 9 of 11)

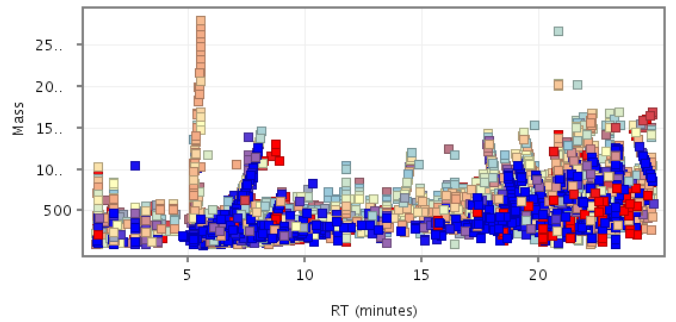
Sample Summary

From the Entities tab, use merging options to manually merge entities. Spectra of selected entities are displayed to help merging.
Compound Frequency tab displays the frequency of aligned compounds across all the samples.
Mass vs RT tab displays a scatter plot of compounds and spreadsheet has the summary of aligned compounds present or absent in individual samples.

Export For Recursion

Total number of Aligned Compounds = **6263**

Entities | Compound Frequency | Mass vs RT



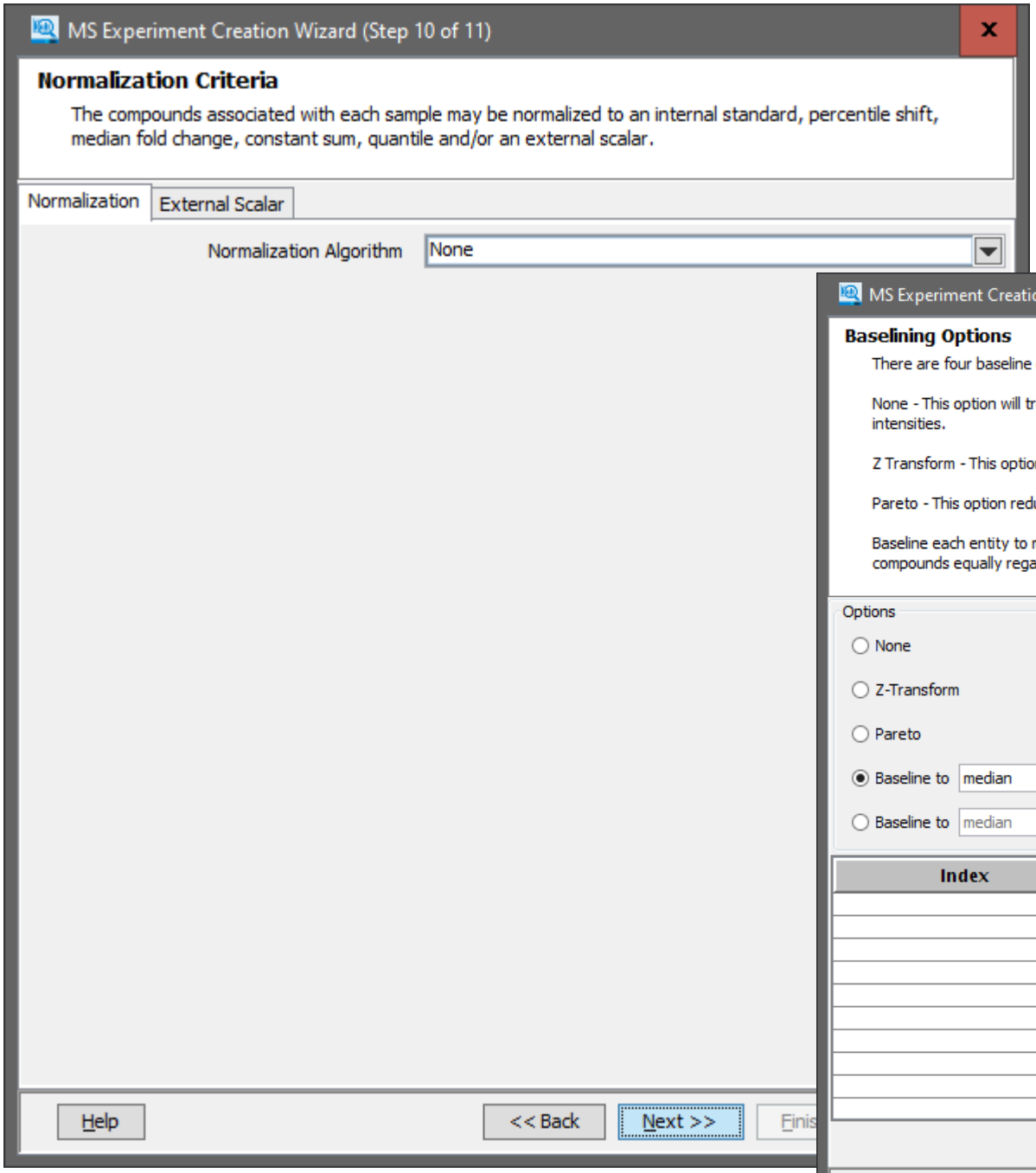
Sample Name	Compounds P...	Compounds A...
Q1	3493	2770
Q2	3728	2535
O1	3556	2707
O2	3760	2503
M1	3945	2318

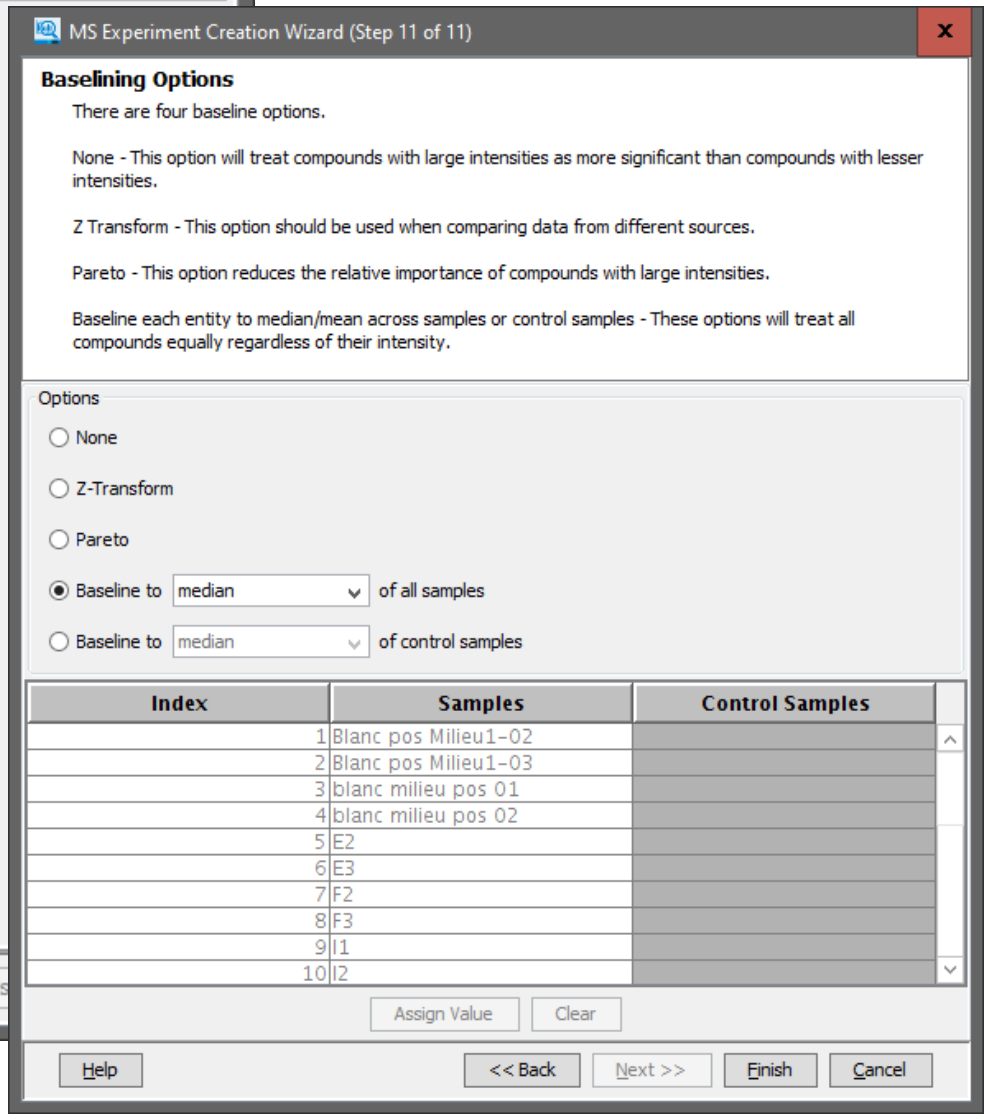
Legend - Mass vs RT

Color by Frequency

3.6 7.5 14 24.4

Help | << Back | Next >> | Finish | Cancel


MS Experiment Creation Wizard (Step 10 of 11)
Normalization Criteria
The compounds associated with each sample may be normalized to an internal standard, percentile shift, median fold change, constant sum, quantile and/or an external scalar.
Normalization
External Scalar
Normalization Algorithm
None
Help
<< Back
Next >>


MS Experiment Creation Wizard (Step 11 of 11)
Baselining Options
There are four baseline options.
None - This option will treat compounds with large intensities as more significant than compounds with lesser intensities.
Z Transform - This option should be used when comparing data from different sources.
Pareto - This option reduces the relative importance of compounds with large intensities.
Baseline each entity to median/mean across samples or control samples - These options will treat all compounds equally regardless of their intensity.
Options
None
Z-Transform
Pareto
Baseline to median of all samples
Baseline to median of control samples
Index
Samples
Control Samples
1 Blanc pos Milieu1-02
2 Blanc pos Milieu1-03
3 blanc milieu pos 01
4 blanc milieu pos 02
5 E2
6 E3
7 F2
8 F3
9 I1
10 I2
Assign Value
Clear
Help
<< Back
Next >>
Finish
Cancel

Workflow Type - Analysis: Significance Testing and Fold Change (Step 1 of 8)

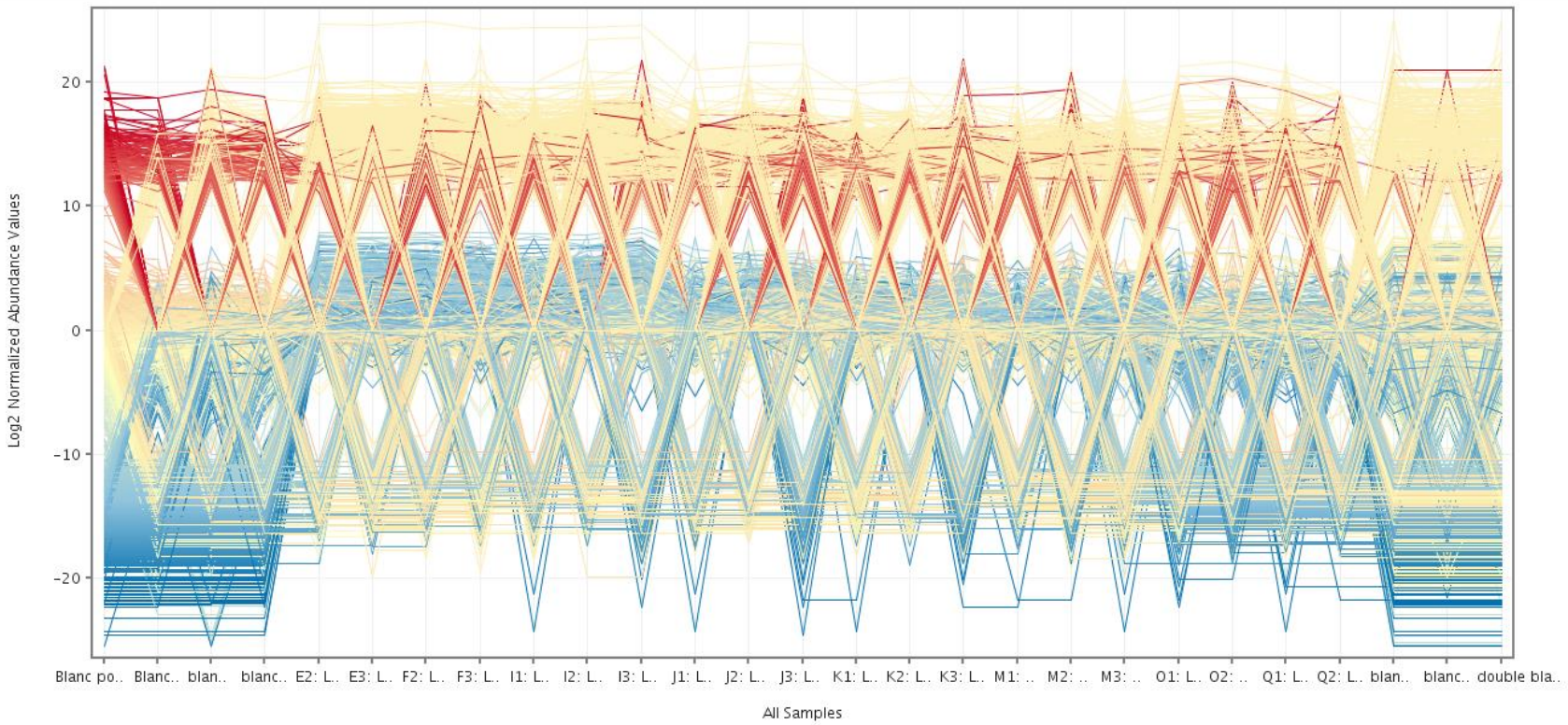
Steps

1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification

Summary Report

The distribution of normalized intensity values across all samples is displayed in the Profile Plot.

MassHunterQual.IDENTIFIED_UNIDENTIFIED_COMPOUNDS experiment, No. of sample(s): **27**



Help | << Back | Next >> | Finish | Cancel

Workflow Type - Analysis: Significance Testing and Fold Change (Step 2 of 8)

Steps

1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification

Experiment Grouping

Experiment parameters define the grouping or replicate structure of your experiment. Enter experiment parameters by clicking on the "Add Parameter" button. You may enter as many parameters as you like, but only the first two parameters will be used for analysis in the guided workflow. Other parameters can be used in the advanced analysis. You can also edit and re-order parameters and parameter values here.
Significance analysis step will be skipped if there are no replicates in any of the condition(s).
Fold change analysis will be skipped if more than one parameter is entered and if the second parameter increases the number of conditions.

Displaying **27** sample(s) with **1** experiment parameter(s). To change, use the button controls below.

Samples	Phaeodactylum.t
Blanc pos Milieu1-02	Media
Blanc pos Milieu1-03	Media
blanc milieu pos 01	Media
blanc milieu pos 02	Media
E2	J0-J1
E3	J0-J1
F2	J0-J1
F3	J0-J1
I1	J4
I2	J4
I3	J4
J1	J5
J2	J5
J3	J5
K1	J6
K2	J6
K3	J6
M1	J8
M2	J8
M3	J8
O1	Jmax10-11
O2	Jmax10-11
Q1	Jmax10-11
Q2	Jmax10-11
blanc meoh pos 02	Blank
blanc meoh pos 03	Blank
double blanc meoh pos 02	Blank

Add Parameter | Edit Parameter | Delete Parameter

Help | << Back | Next >> | Finish | Cancel

Workflow Type - Analysis: Significance Testing and Fold Change (Step 3 of 8)

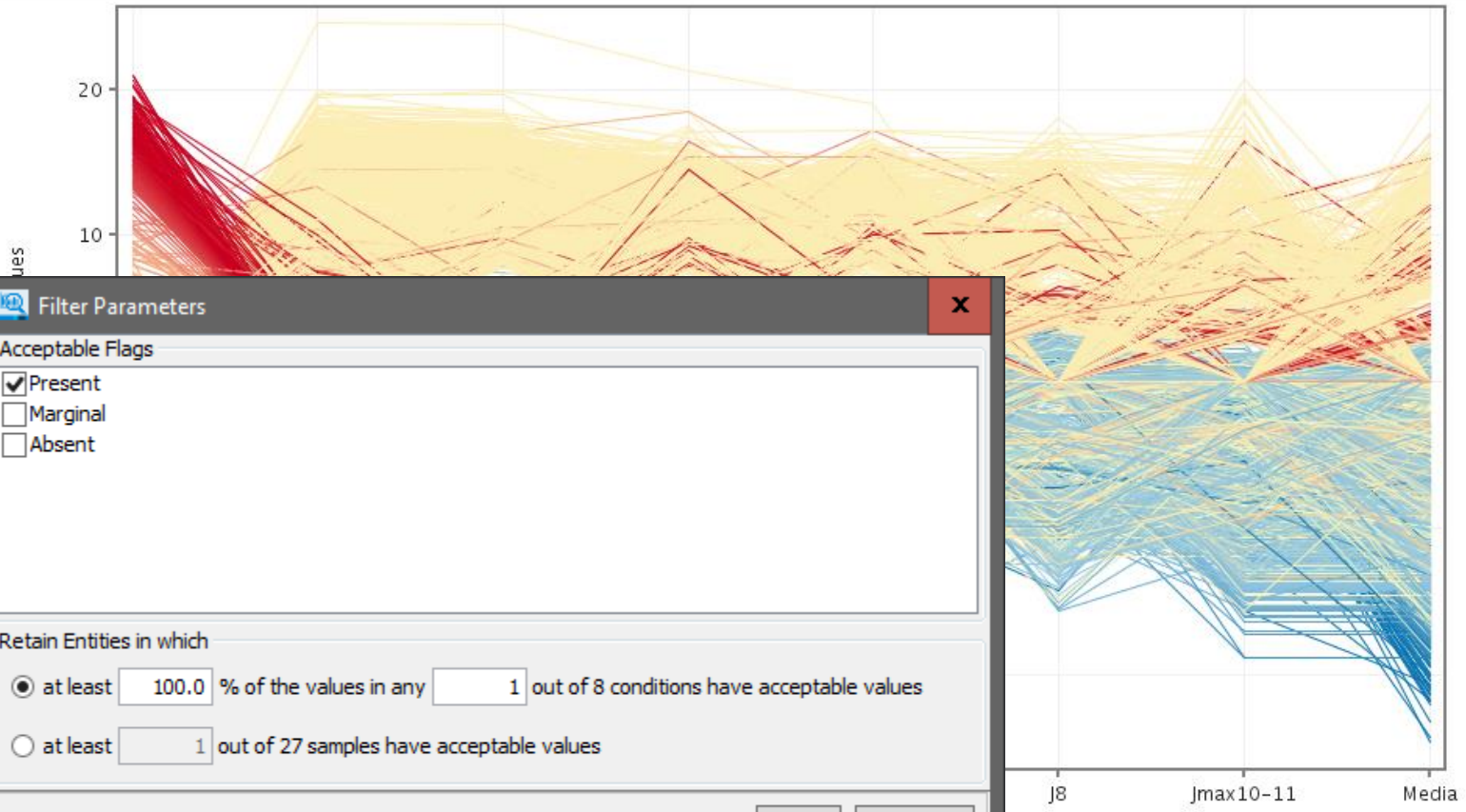
Steps

1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification

Filter Flags

If flag values are present, entities are filtered based on their flag values. Otherwise, entities are filtered based on their signal intensity values. To change the filter criteria, click on the "Re-run Filter" button.

Displaying **6263** out of **6263** entities where atleast **1** out of **27** samples have flags in **[P, M]**.



Filter Parameters

Acceptable Flags

- [x] Present
- [ ] Marginal
- [ ] Absent

Retain Entities in which

- (•) at least 100.0 % of the values in any 1 out of 8 conditions have acceptable values
- ( ) at least 1 out of 27 samples have acceptable values

OK Cancel

Re-run Filter

Help << Back Next >> Finish Cancel

Workflow Type - Analysis: Significance Testing and Fold Change (Step 3 of 8)

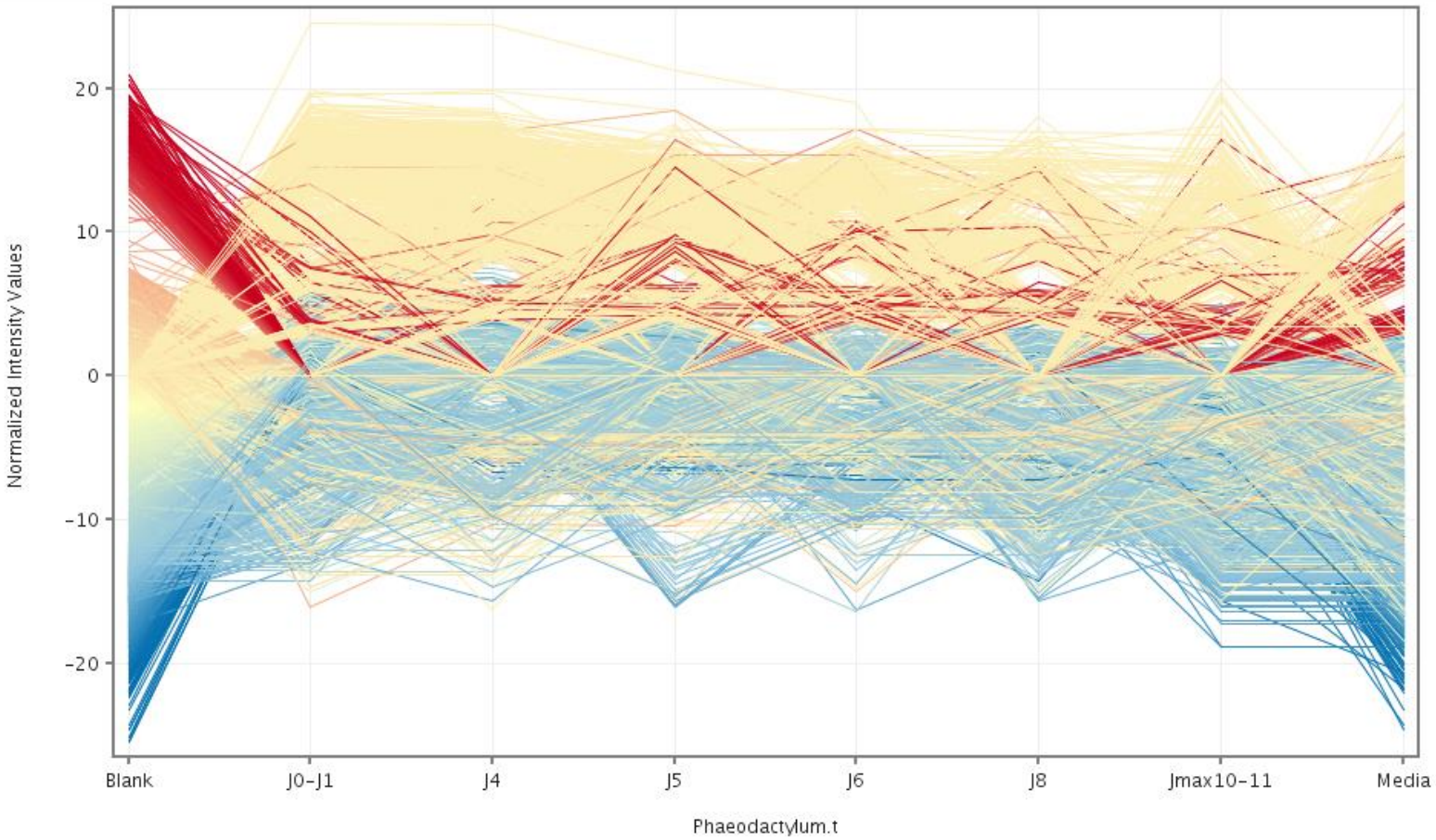
Steps

1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification

Filter Flags

If flag values are present, entities are filtered based on their flag values. Otherwise, entities are filtered based on their signal intensity values. To change the filter criteria, click on the "Re-run Filter" button.

Displaying **5427** out of **6263** entities where atleast **100.0** percent of samples in any **1** out of **8** conditions have flags in **[P]**.



Re-run Filter

Help

<< Back | Next >> | Finish | Cancel

Workflow Type - Analysis: Significance Testing and Fold Change (Step 4 of 8)

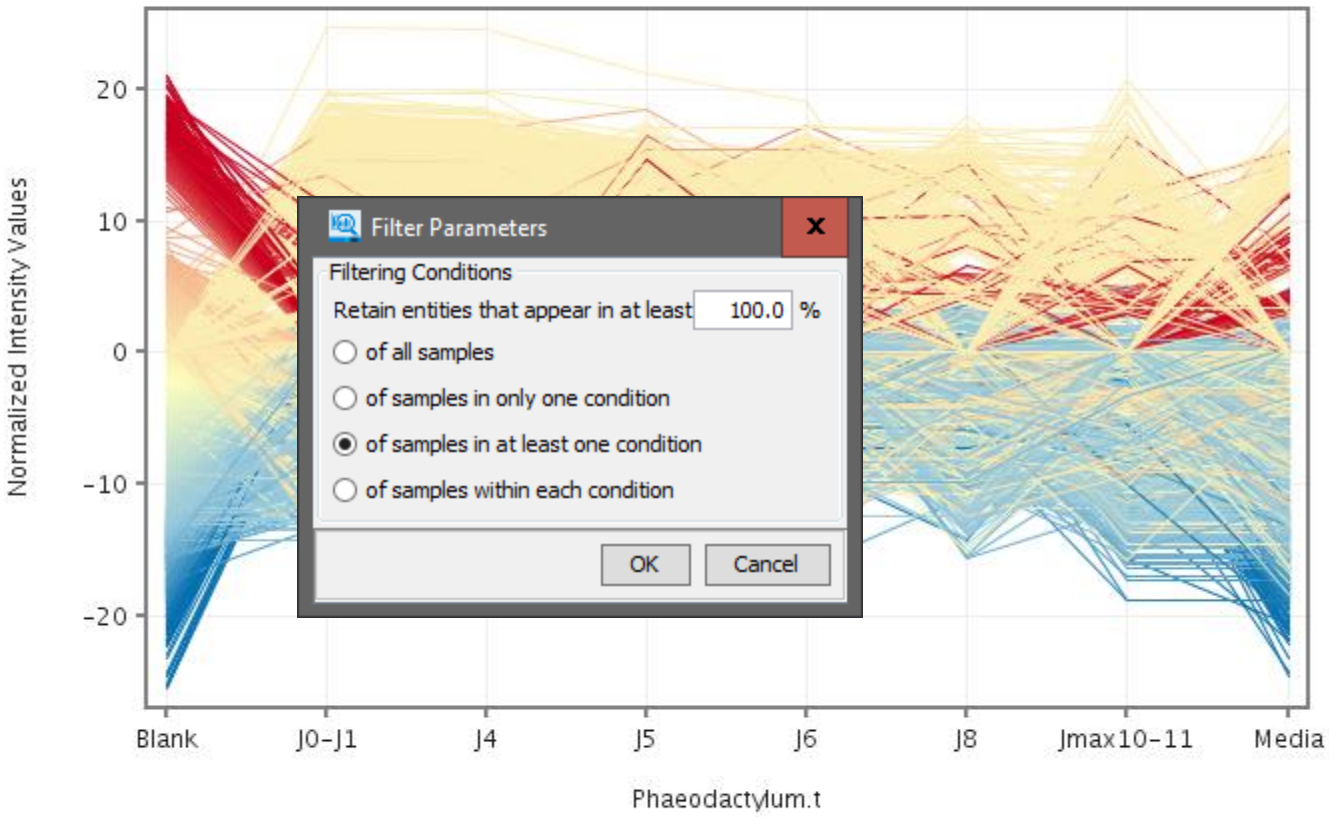
Steps

1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification

Filter By Frequency

Entities are filtered based on their Frequency of occurance across samples. Define the stringency of the filter by selecting the minimum percentage of samples in which entity must pass the filter or by selecting the minimum percentage of samples within any x out of y conditions in which the entity must pass the filter. To change the filter criteria, click on the "Re-run Filter" button.

Displaying **5427** of **5427** entities where at least 100.0 percent of samples in any 1 out of 8 conditions has flag **P**



Filter Parameters

Filtering Conditions

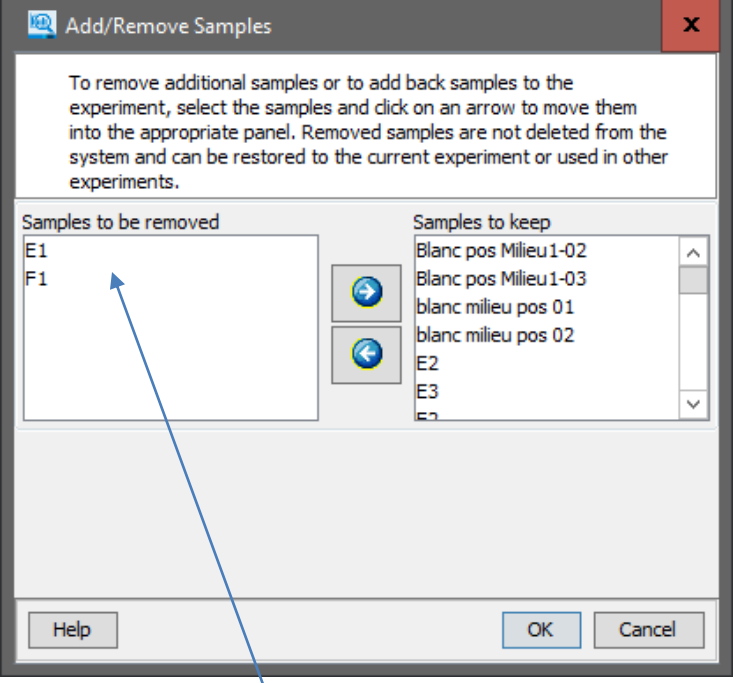
Retain entities that appear in at least 100.0 %

- of all samples
- of samples in only one condition
- of samples in at least one condition
- of samples within each condition

OK Cancel

Re-run Filter

Help << Back Next >> Finish Cancel



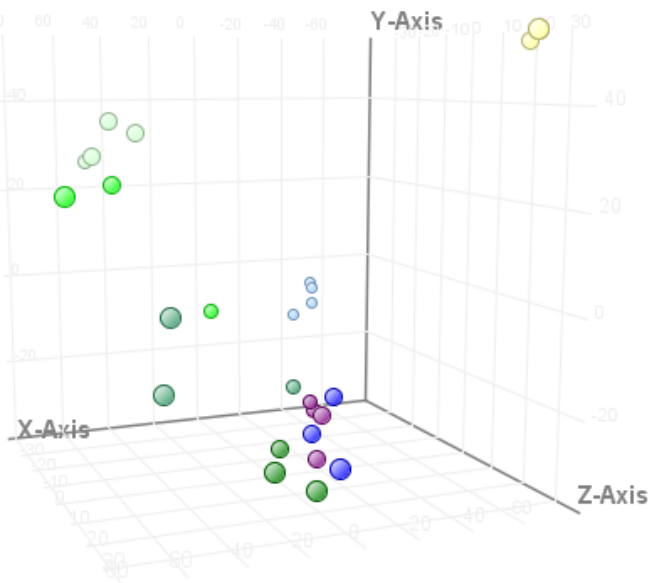
Legend - 3D PCA Scores

Color by Diatom Pt

- Media
- J0-J1
- J4
- J5
- J6
- J8
- Jmax10-11
- Blank

Description

Algorithm: Principal Components Analysis
Parameters:
Column indices = [1-27]
Pruning option = [numPrincipalComponents, [4]]
Mean centered = true
Scale = true
3-D scores = true
PCA on = Columns



X-Axis Component 1 (33.1%)

Y-Axis Component 2 (13.36%)

Z-Axis Component 3 (7.78%)

Workflow Type - Analysis: Significance Testing and Fold Change (Step 5 of 8)

Steps

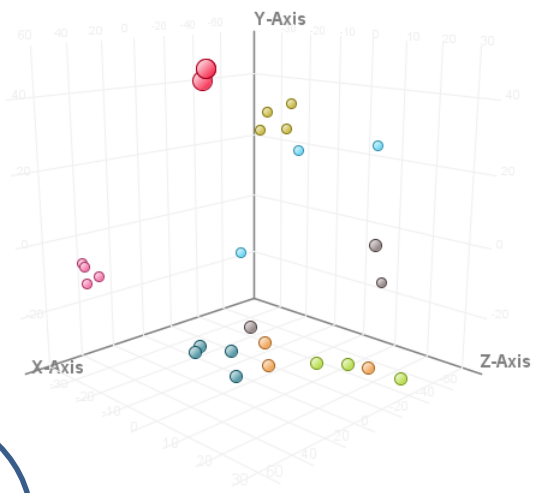
1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification

QC on samples

Sample quality can be assessed by examining the values in the PCA plot and other experiment specific quality plots.

Displaying **27** out of **27** samples retained in the analysis.

Samples	Phaeodactylum.t
Blanc pos Milieu1-02	Media
Blanc pos Milieu1-03	Media
blanc milieu pos 01	Media
blanc milieu pos 02	Media



X-Axis Component 1 (36.53%)

Y-Axis Component 2 (14.76%)

Z-Axis Component 3 (8.18%)

Legend - 3D PCA Scores

Color by Phaeodactylum.t

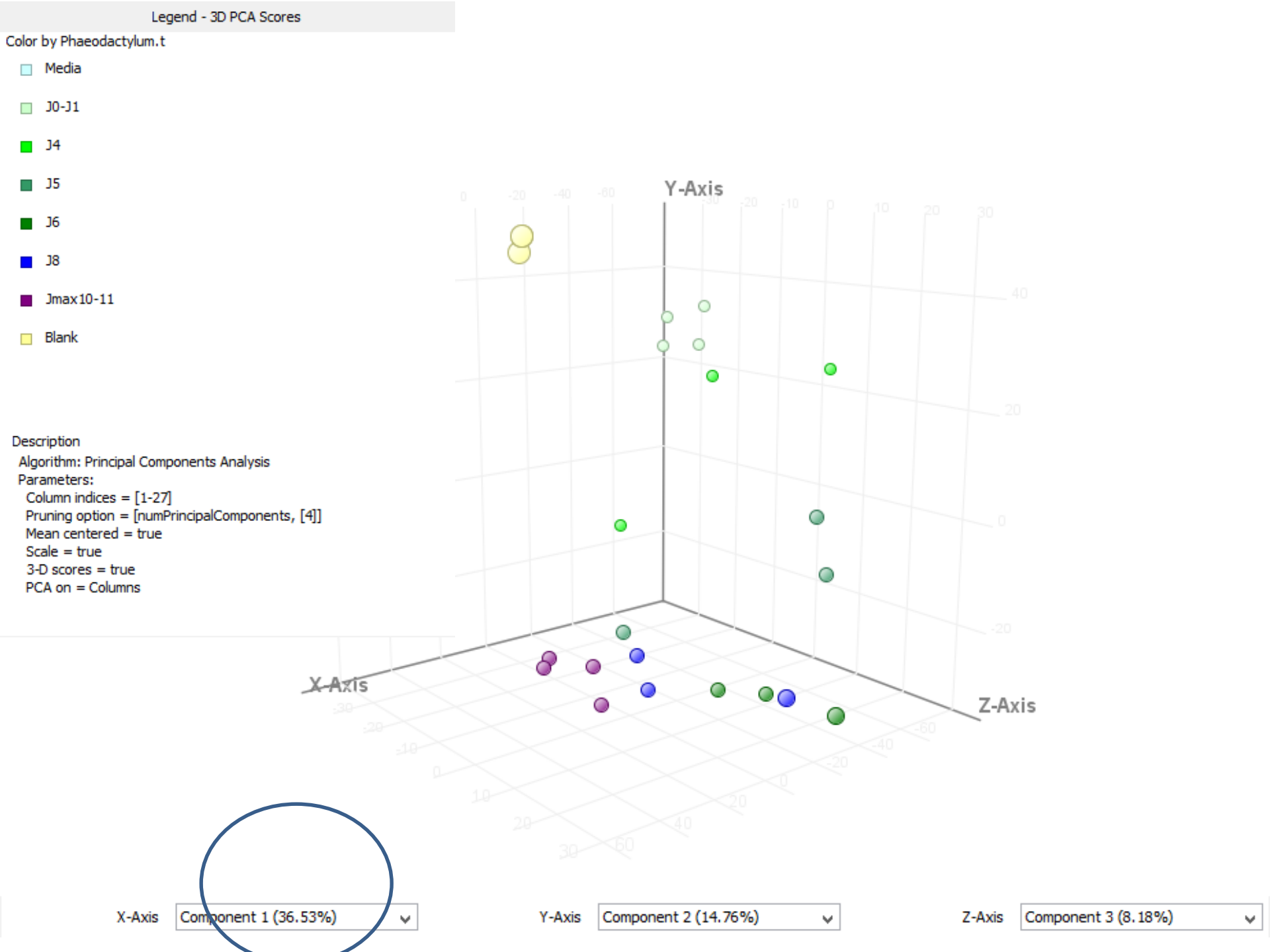
- Media
- J0-J1
- J4
- J5
- J6
- J8
- Jmax10-11
- Blank

Description

Algorithm: Principal Components Analysis
Parameters:
Column indices = [1-27]
Pruning option = [numPrincipalComponents, [4]]
Mean centered = true
Scale = true
3-D scores = true
PCA on = Columns

Help

<< Back | Next >> | Finish | Cancel


Legend - 3D PCA Scores
Color by Phaeodactylum.t
Media
J0-J1
J4
J5
J6
J8
Jmax10-11
Blank
Description
Algorithm: Principal Components Analysis
Parameters:
Column indices = [1-27]
Pruning option = [numPrincipalComponents, [4]]
Mean centered = true
Scale = true
3-D scores = true
PCA on = Columns
Y-Axis
X-Axis
Z-Axis
X-Axis
Component 1 (36.53%)
Y-Axis
Component 2 (14.76%)
Z-Axis
Component 3 (8.18%)

nificance Analysis

Entities are filtered based on their p-values calculated from statistical analysis. To apply the new p-value cut-off, drag the "p-value cut-off" slider or input the new cut-off value in the text box. You will not be able to proceed to the next step if no entities pass the filter.

Displaying **3886** out of **5007** entities satisfying corrected p-value cut-off **0.05**.

Description

ted Test:	Oneway ANOVA
ue computation:	Asymptotic
ple Testing Correction:	Benjamini-Hochberg

t Summary

	P all	P < 0.05	P < 0.02	P < 0.01	P < 0.005	P < 0.001
cted p-value	5007	3886	3578	3357	3157	2662
cted by chance		194	71	33	15	2

Compound	p	p (Corr)
4331@21.596006	1.50E-11	7.21E-11
4975@22.528994	2.00E-09	8.24E-09
3388@23.494001	1.26E-08	4.86E-08
0877@10.224	4.34E-04	8.29E-04
1234@20.155005	9.70E-20	6.29E-19
5234@22.405006	8.78E-10	3.74E-09
0627@21.367002	7.89E-20	5.16E-19
5243@23.028994	8.63E-12	4.17E-11
4288@22.243006	3.49E-12	1.71E-11
568@21.394005	1.31E-05	3.31E-05
4647@22.251005	1.63E-10	7.42E-10
5491@22.372002	4.10E-25	4.63E-24
1593@22.719994	5.27E-18	3.08E-17
1861@22.719994	3.11E-17	1.75E-16
5498@22.288002	5.64E-10	2.47E-09
5647@23.453001	1.27E-11	6.11E-11
1962@3.871	4.45E-28	8.02E-27

p-value cut-off 0.05

<< Back | Next >> | Finish | Cancel

Workflow Type - Analysis: Significance Testing and Fold Change (Step 7 of 8)

Steps

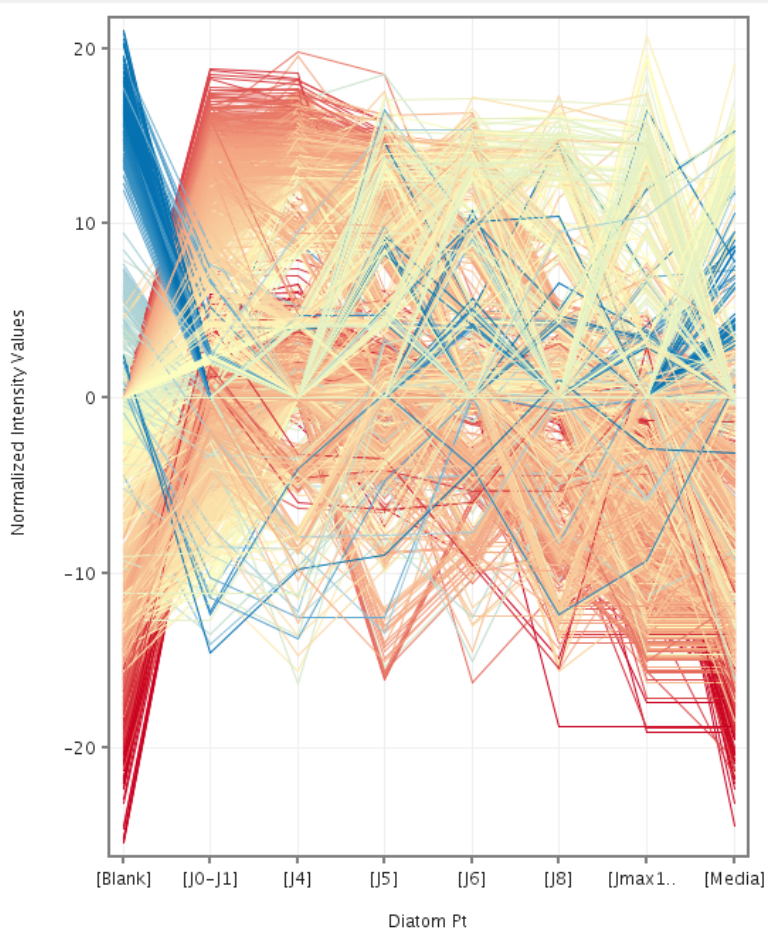
1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification

Fold Change

Compounds that satisfy a fold change cut-off of 2.0 in at least one condition pair are displayed by default. To apply the new fold change cut-off, drag the "Fold change cut-off" slider or input the new cut-off value in the text box.

Displaying **3802** out of **3886** entities with fold change cut-off of **2.0** in **1** out of **7** condition pairs with **[Blank]** as the control condition.

Compou...	FC ([J0-J...	FC ([J4] v...	FC ([J5] v...	FC ([J6] v...	FC ([J8] v...	FC ([Jma...	FC ([Med...
132.069...	58.76	122.27	88.91	63.76	93.18	27.76	86.08
658.423...	661081...	989430...	698760...	726438...	394614...	111128...	3456.88
829.586...	268338...	461864...	145766...	409832...	425429...	204831...	-1.00
610.161...	-64.44	-68.68	-72.34	-66.64	-67.05	-67.43	-60.71
790.464...	520715...	628692...	553820...	537812...	428885...	142050...	1829.25
180.095...	142021...	158042...	923467...	845459...	788047...	417066...	863941...
337.175...	431414...	360357...	750848...	166738...	534447...	169754...	45.18
325.371...	1.27	1.44	1.42	2.00	1.41	4.42	-1.24
785.508...	319757...	397335...	335121...	321720...	248327...	922145...	2320.91
792.479...	130647...	258330...	138306...	726004...	307132...	784933...	94.57
558.124...	-59.37	-76.74	-68.93	-61.97	-56.89	-53.35	-41.32
658.424...	661381...	989336...	698764...	726476...	394419...	111258...	3355.73
370.094...	-81.82	-81.03	-81.35	-80.66	-85.44	-89.01	-82.76
803.569...	921374...	152439...	205762...	169724...	968203...	351040...	-1.00
658.423...	670394...	146555...	840438...	575653...	213259...	478684...	12.06
273.180...	251279...	237603...	253917...	537409...	174645...	67020.03	-1.00
520.222...	578949...	404491...	191464...	190736...	162741...	567048...	154234...
678.504...	1112.71	935.18	927.89	1001.81	1208.79	989.38	662.56
330.313...	-231.91	-183.44	-235.06	-93.13	-79.05	-179.87	-611.26
580.392...	115907...	213769...	121019...	124161...	466603...	826378...	75.51
536.141...	-49.70	-51.11	-50.79	-49.19	-51.19	-52.71	-52.79
658.424...	826718...	147964...	965842...	888279...	401553...	987771...	641.84
185.106...	583540...	632388...	844174...	620992...	600222...	945819...	118500...
750.528...	135379...	185003...	64463.14	8639.14	173.20	616487...	-1.00
418.365...	-57.74	-40.39	-58.83	-29.90	-34.79	-74.68	-186.89
287.196...	155816...	197113...	410645...	996777...	287491...	88931.02	-1.00
567.470...	-19.93	-13.60	-19.86	-14.91	-19.13	-28.81	-150.18
479.418...	-31.75	-23.48	-35.20	-20.47	-25.19	-46.23	-109.25
300.277...	-1.05	-1.10	1.11	-1.05	-1.06	50.00	-1.17
738.433...	858436...	152235...	632158...	136156...	254995...	46627.55	8.48
611.497...	-19.01	-12.92	-18.33	-14.22	-18.48	-25.08	-158.49
374.338...	-110.49	-77.34	-125.40	-51.37	-48.21	-119.87	-272.61
257.087...	21831.80	140597...	87961.66	78830.70	66580.66	33672.20	67919.78
462.123...	-45.36	-48.32	-42.22	-43.81	-52.95	-51.64	-49.94
655.523...	-19.79	-13.34	-18.47	-14.98	-18.68	-23.18	-173.31
354.062...	-95.08	-96.32	-97.01	-94.22	-99.04	-102.70	-99.23
787.524...	968401...	160218...	974358...	655051...	343649...	107508...	9.67
606.428...	991196...	167770...	106766...	954276...	507386...	743783...	8.54
755.568...	253244...	473776...	471023...	475124...	876277...	33.58	-1.00
790.464...	521379...	628743...	553869...	537939...	428966...	142050...	129.76
956.549...	809485...	128103...	836860...	604251...	314127...	977679...	-1.00



Fold change cut-off 2.0

Minimum no. of pairs 1

Control Group Blank

Help

<< Back | Next >> | Finish | Cancel

Workflow Type - Analysis: Significance Testing and Fold Change (Step 7 of 8)

Steps

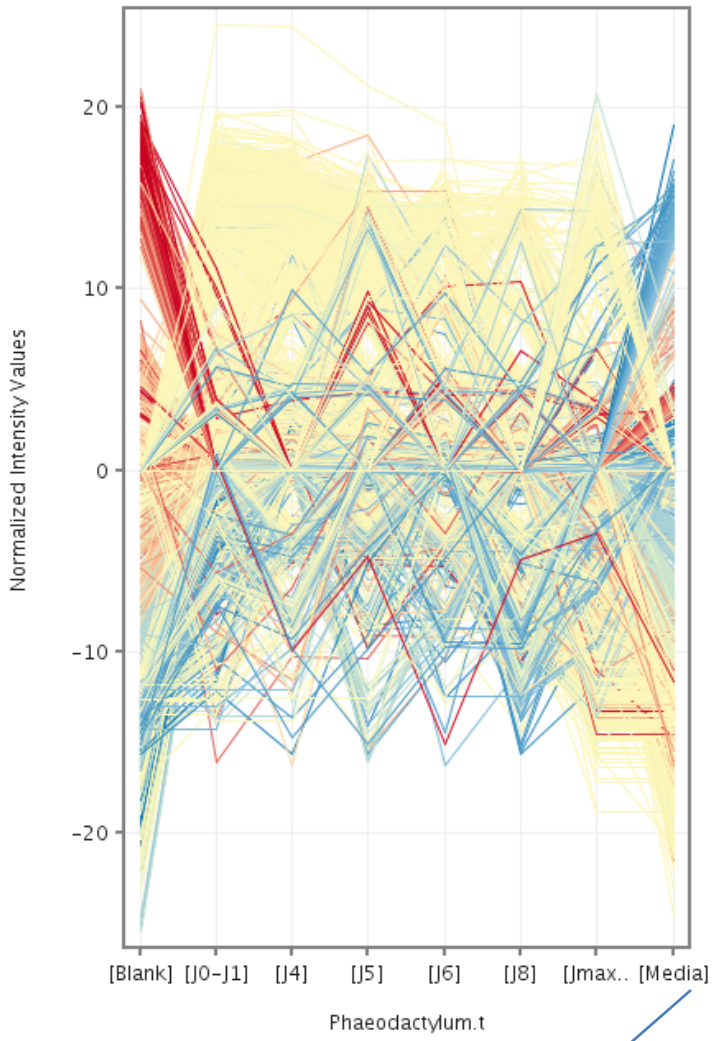
1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification

Fold Change

Compounds that satisfy a fold change cut-off of 2.0 in at least one condition pair are displayed by default. To apply the new fold change cut-off, drag the "Fold change cut-off" slider or input the new cut-off value in the text box.

Displaying **4280** out of **4418** entities with fold change cut-off of **2.0** in **1** out of **7** condition pairs with **[Media]** as the control condition.

Compou...	FC ([Blan...	FC ([J0-J...	FC ([J4] v...	FC ([J5] v...	FC ([J6] v...	FC ([J8
132.069...	-86.08	-2.22	1.42	1.03	-1.35	
658.423...	-3456.88	30281.97	28622.04	20213.57	21014.28	1141
829.586...	-1.00	458669...	461864...	145766....	409832...	4254
610.161...	60.71	-1.10	-1.13	-1.19	-1.10	-
790.464...	-1829.25	33062.43	34368.84	30275.80	29400.67	2344
180.095...	-863941...	-28.27	1.83	1.07	-1.02	-
337.175...	-45.18	101141...	797537....	166176....	36902.20	1182
325.371...	1.24	1.77	1.78	1.76	2.48	
785.508...	-2320.91	16479.46	17119.79	14439.21	13861.82	1069
792.479...	-94.57	217777....	273164....	146248....	76769.25	3247
558.124...	41.32	-1.54	-1.86	-1.67	-1.50	-
658.424...	-3355.73	31217.08	29482.04	20823.04	21648.86	1175
370.094...	82.76	-1.02	1.02	1.02	1.03	-
803.569...	-1.00	137468...	152439...	205762...	169724...	9682
658.423...	-12.06	133773...	121572...	697167....	477520....	17690
273.180...	-1.00	264387...	237603...	253917...	537409....	17464
520.222...	-154234...	3.64	26.23	12.41	12.37	1
678.504...	-662.56	1.60	1.41	1.40	1.51	
330.313...	611.26	3.45	3.33	2.60	6.56	
580.392...	-75.51	311446....	283090....	160263....	164425....	6179
536.141...	52.79	1.02	1.03	1.04	1.07	
658.424...	-641.84	22330.08	23052.99	15047.94	13839.49	625
185.106...	-118500...	-47.12	-18.74	-14.04	-19.08	-1
750.528...	-1.00	128262...	185003...	64463.22	8639.16	17
418.365...	186.89	4.21	4.63	3.18	6.25	
287.196...	-1.00	173931...	197113...	410645...	996777....	28749
567.470...	150.18	10.56	11.04	7.56	10.07	
479.418...	109.25	4.42	4.65	3.10	5.34	
300.277...	1.17	1.14	1.06	1.30	1.11	
738.433...	-8.48	184522...	179601...	745797....	160632....	3008
611.497...	158.49	11.90	12.27	8.65	11.14	
374.338...	272.61	3.15	3.52	2.17	5.31	
257.087...	-67919.78	-16.92	2.07	1.30	1.16	-
462.123...	49.94	1.10	1.03	1.18	1.14	-
655.523...	173.31	12.62	12.99	9.38	11.57	
354.062...	99.23	1.02	1.03	1.02	1.05	
787.524...	-9.67	143676...	165666...	100749...	677326....	35533
606.428...	-8.54	188443...	196443...	125013...	111736...	59410



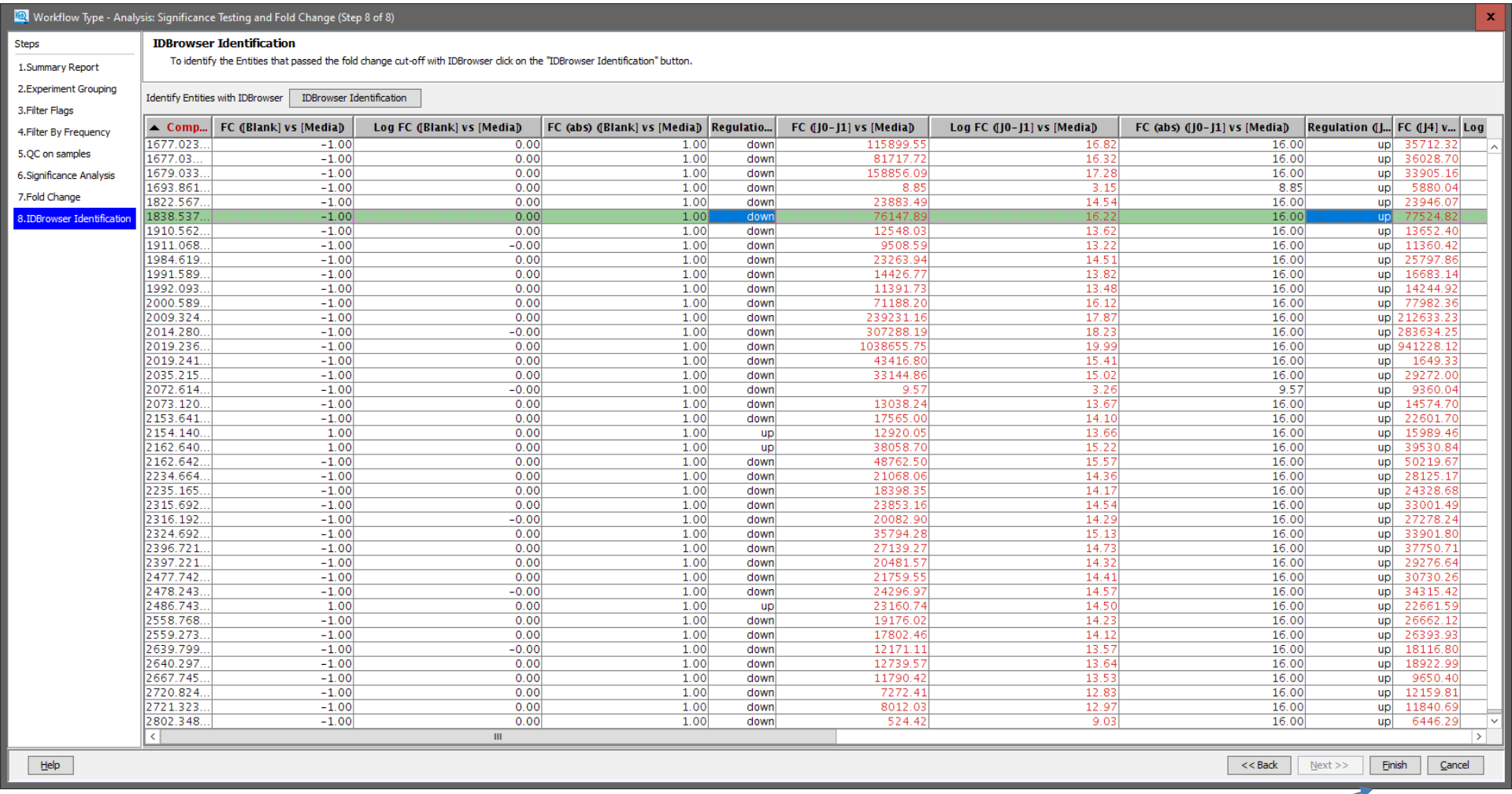
Fold change cut-off 2.0

Minimum no. of pairs 1

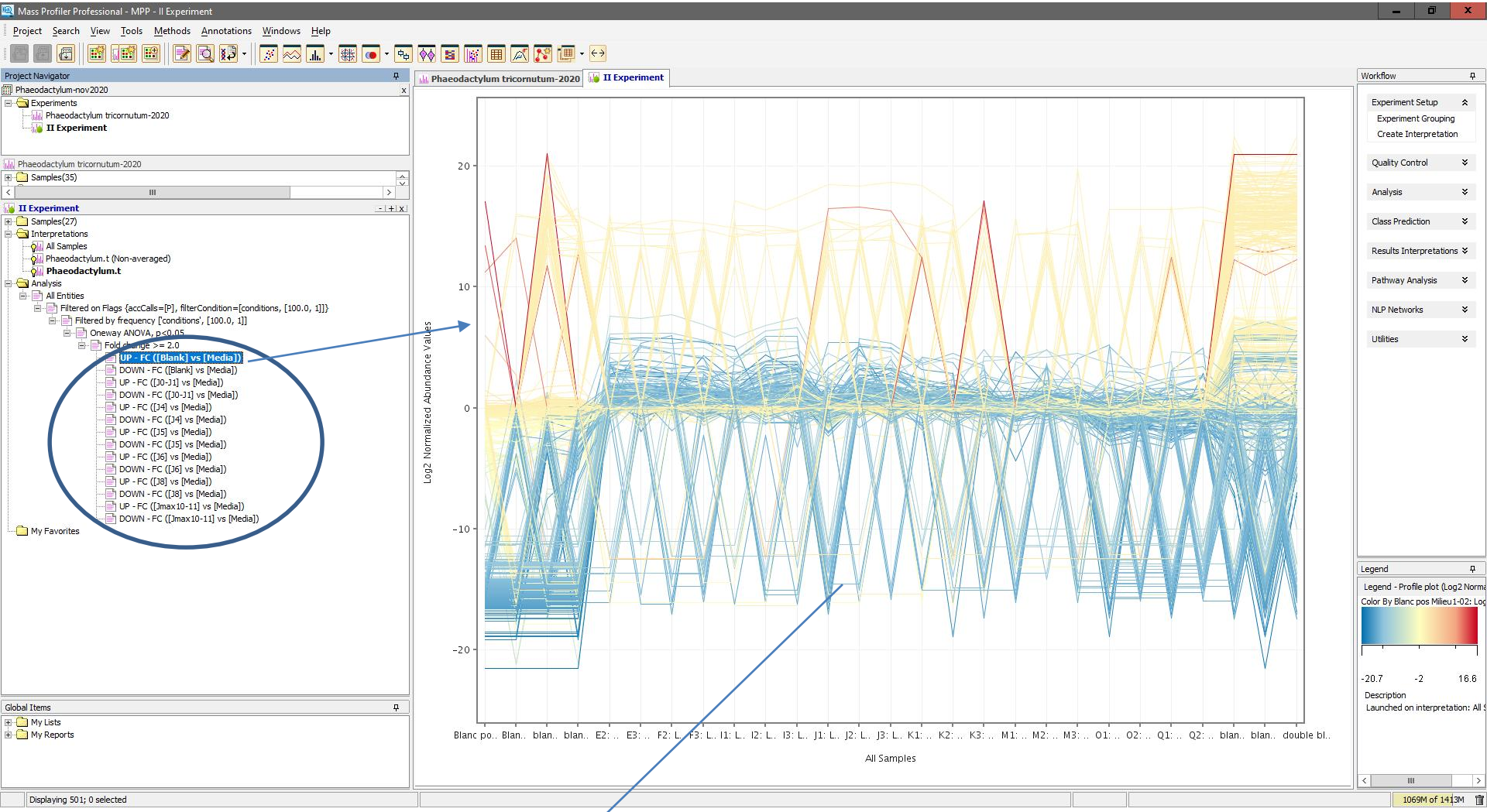
Control Group Media

Help

<< Back | Next >> | Finish | Cancel

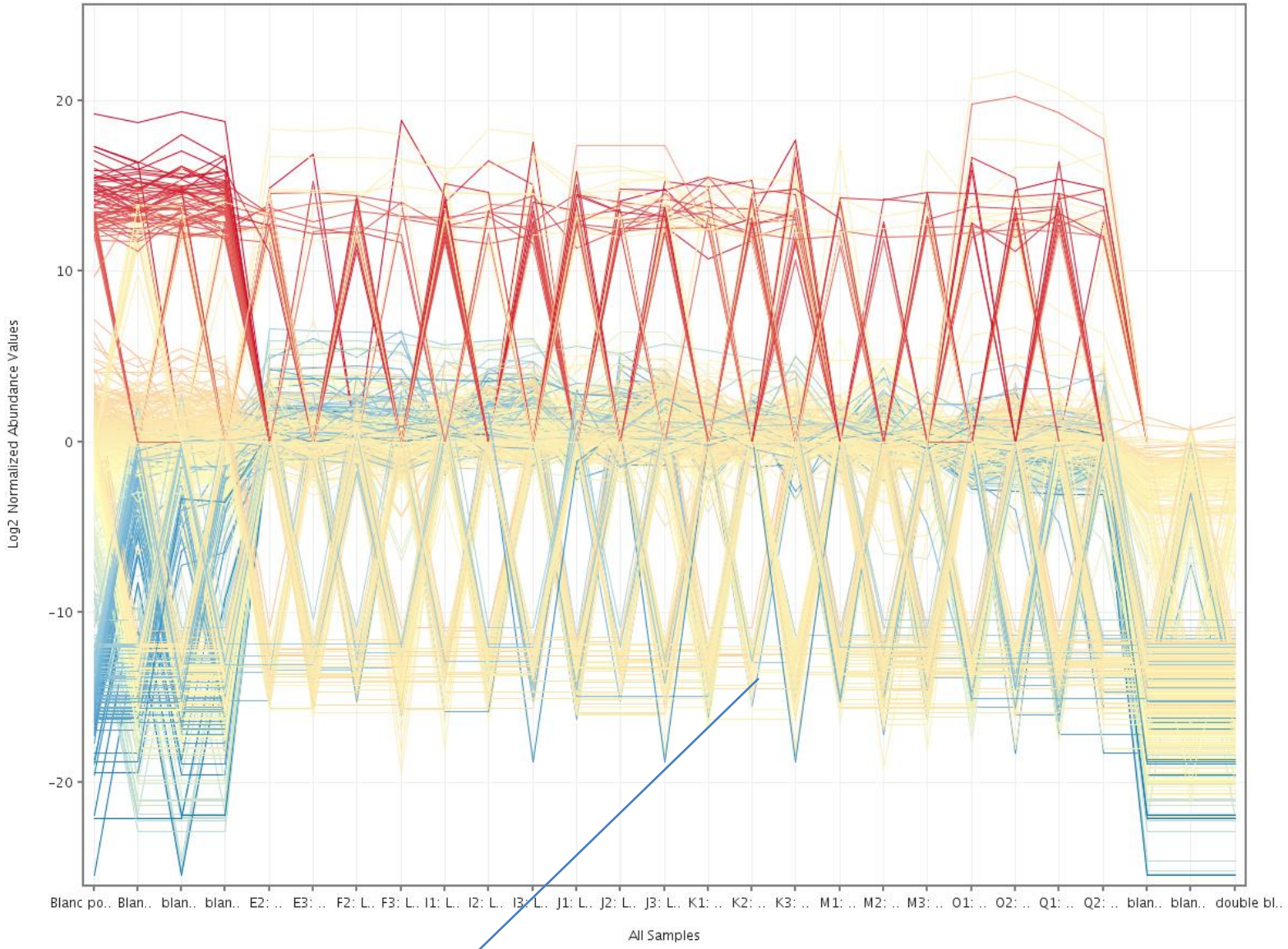


Fichier exporté dans Excel et envoyé chez vous



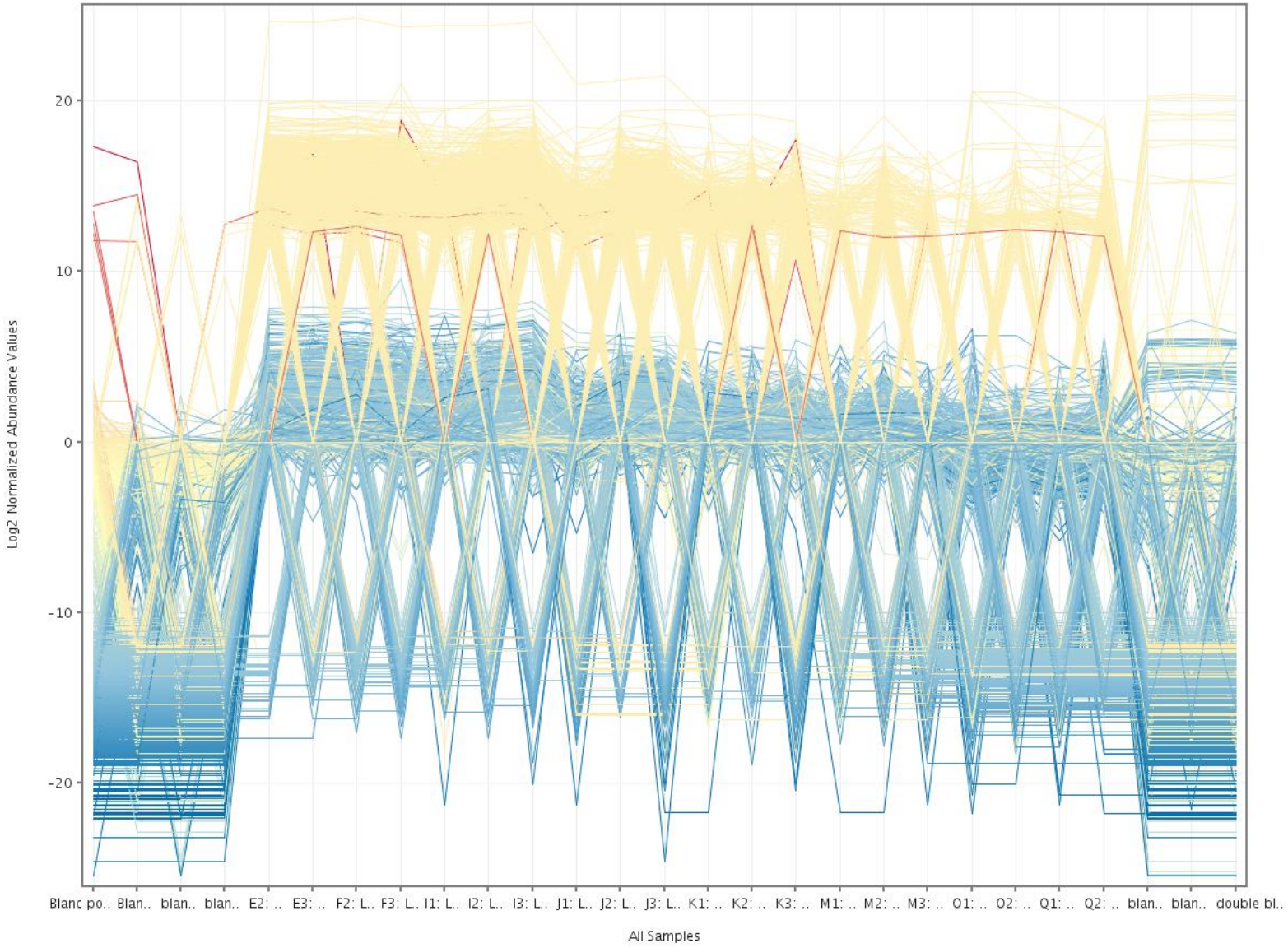
On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 501 métabolites UP - FC ([Blank] vs [Media])



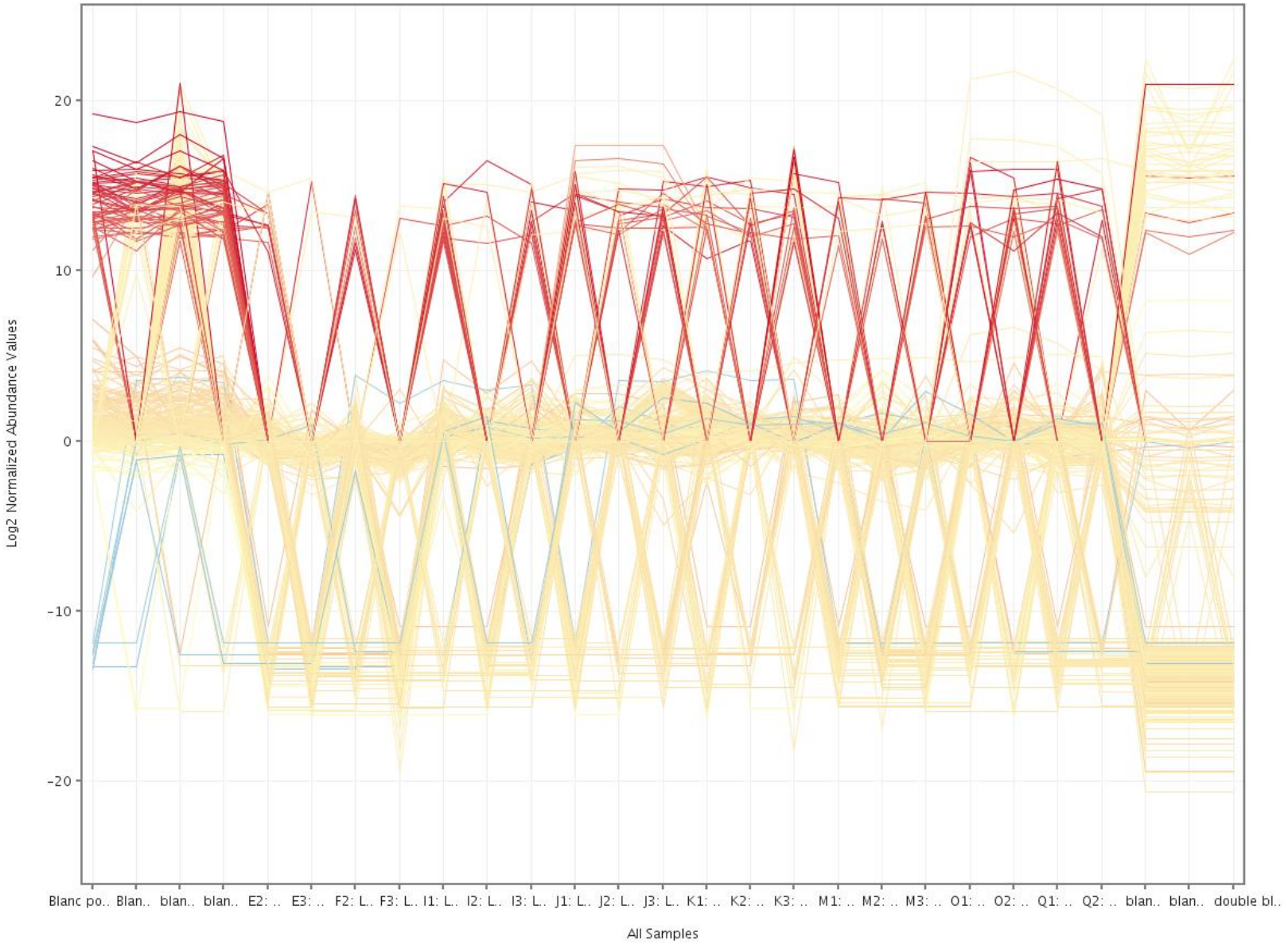
On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 1381 métabolites DOWN - FC ([Blank] vs [Media])



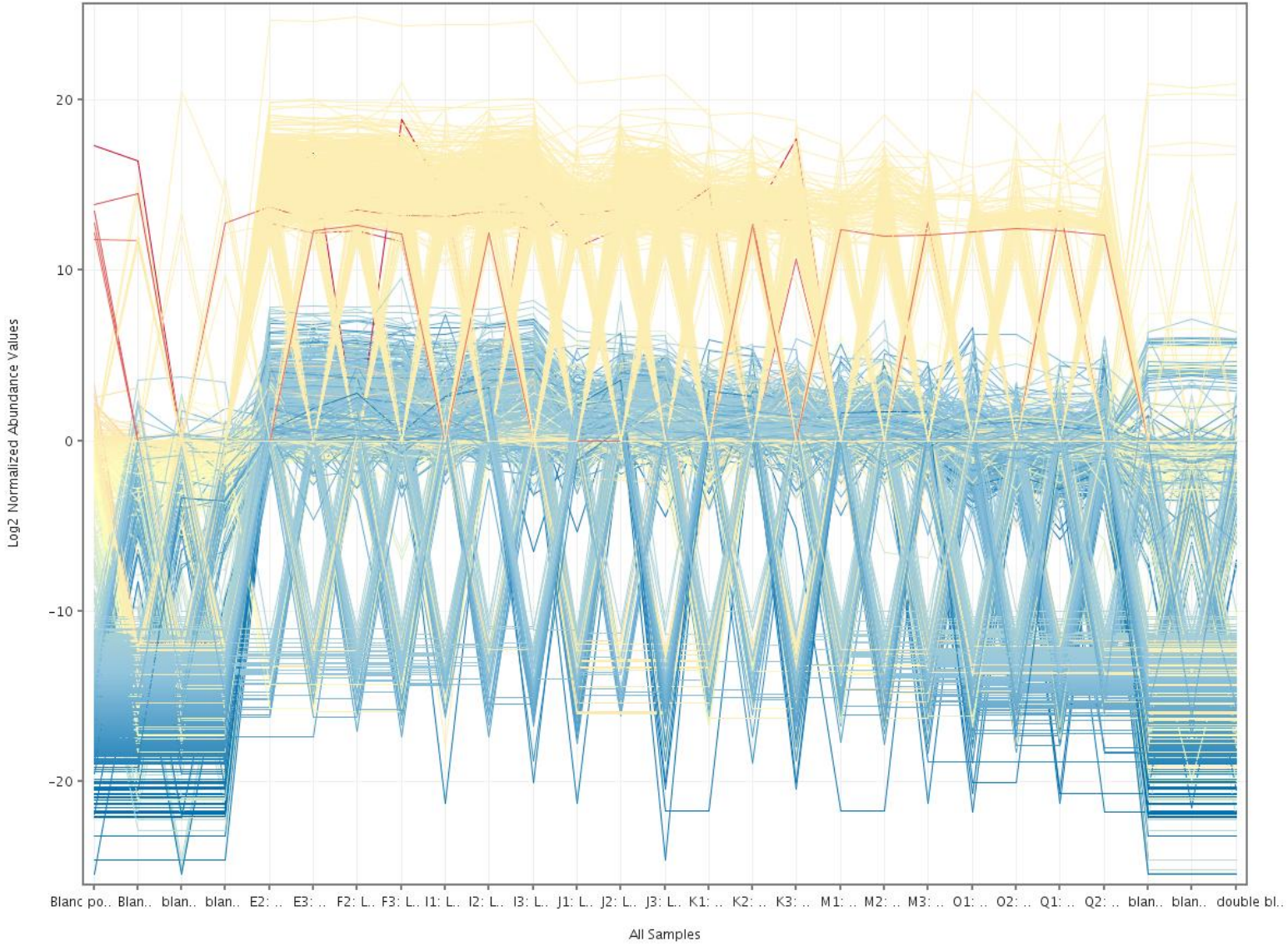
On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 2956 métabolites UP - FC ([J0-J1] vs [Media])



On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

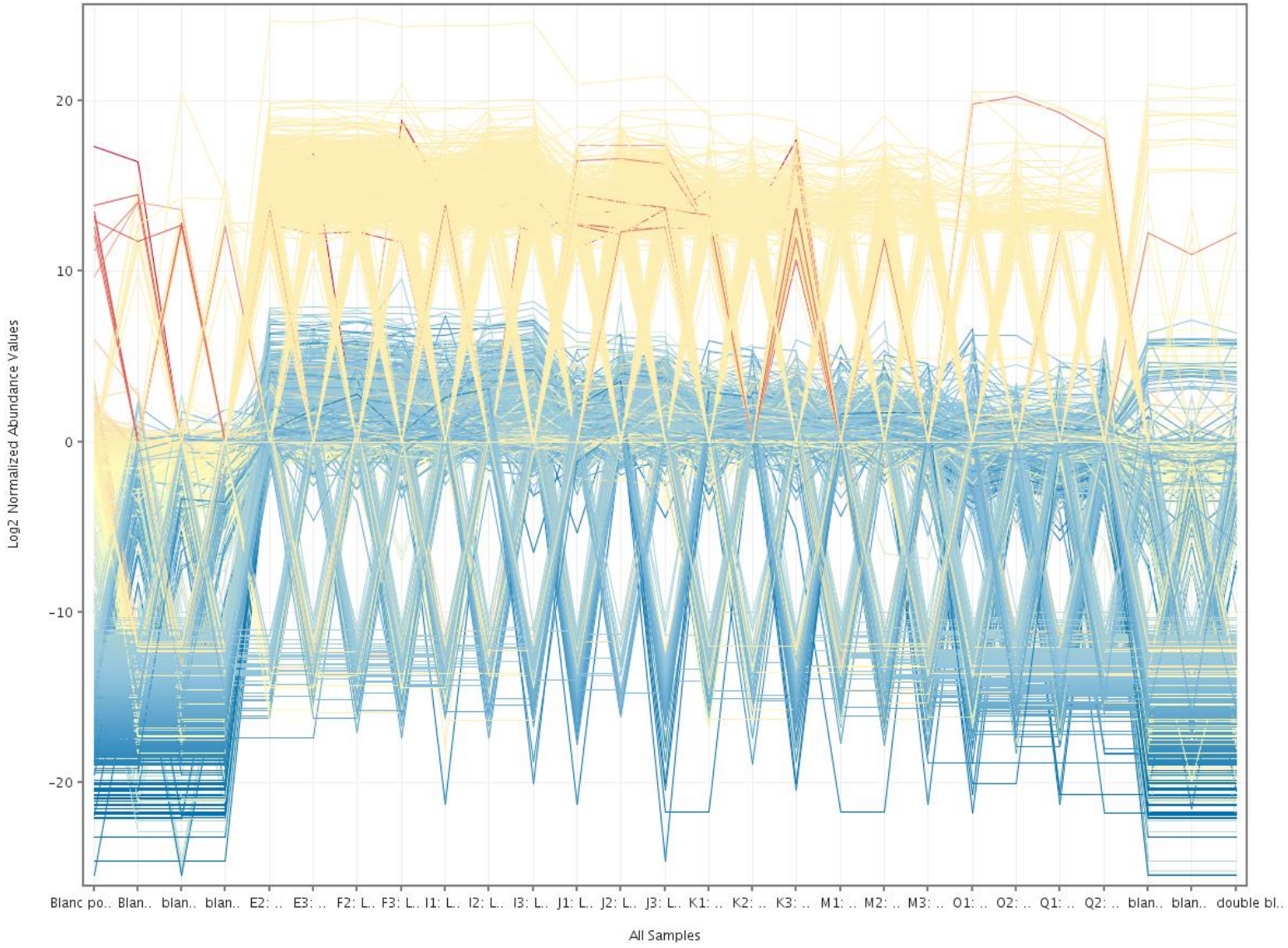
Ici les 378 métabolites DOWN - FC ([J0-J1] vs [Media])



On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

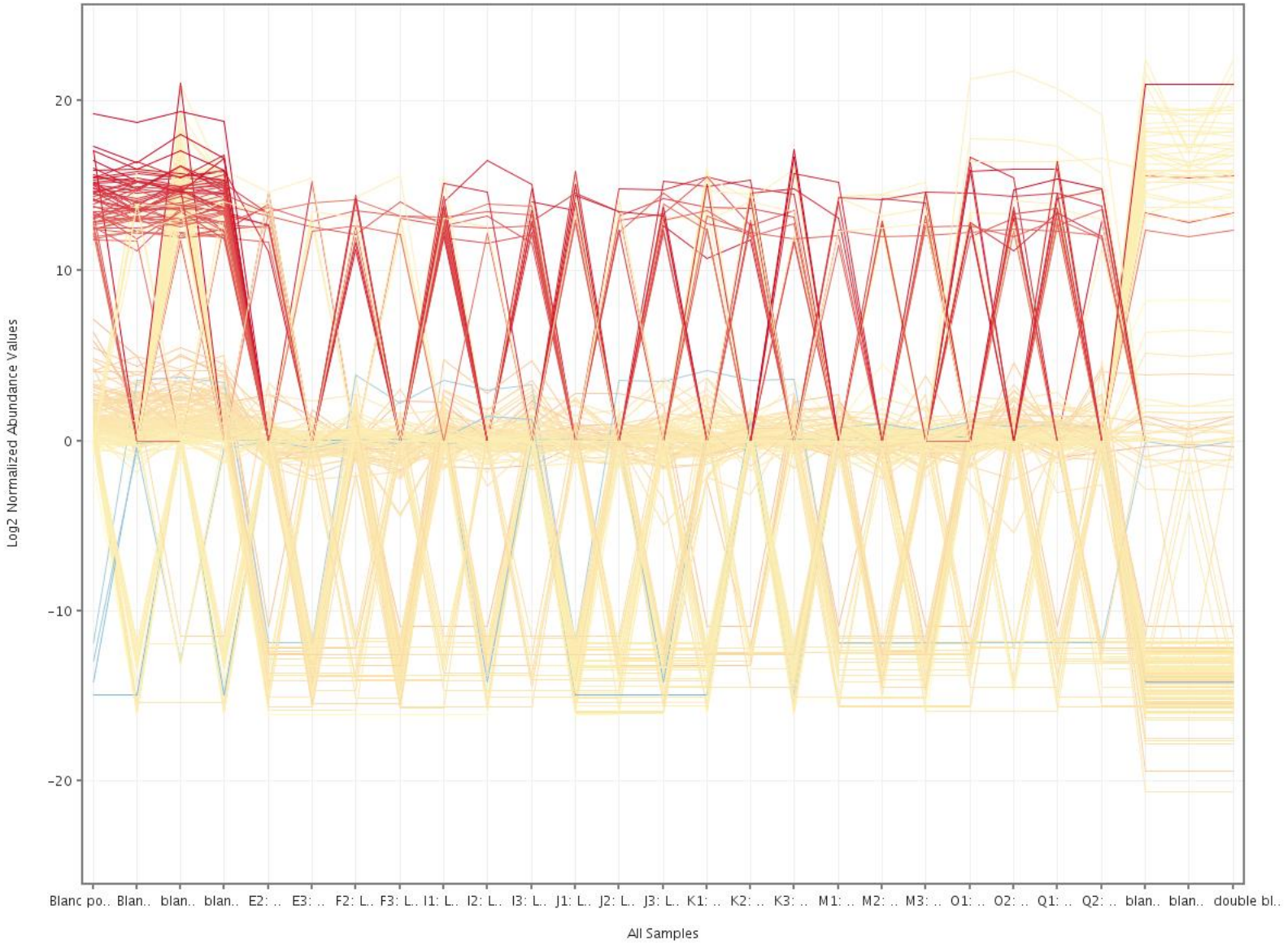
Ici les 3048 métabolites UP - FC ([J4] vs [Media])

On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé
Ici les 272 métabolites DOWN - FC ([J4] vs [Media])



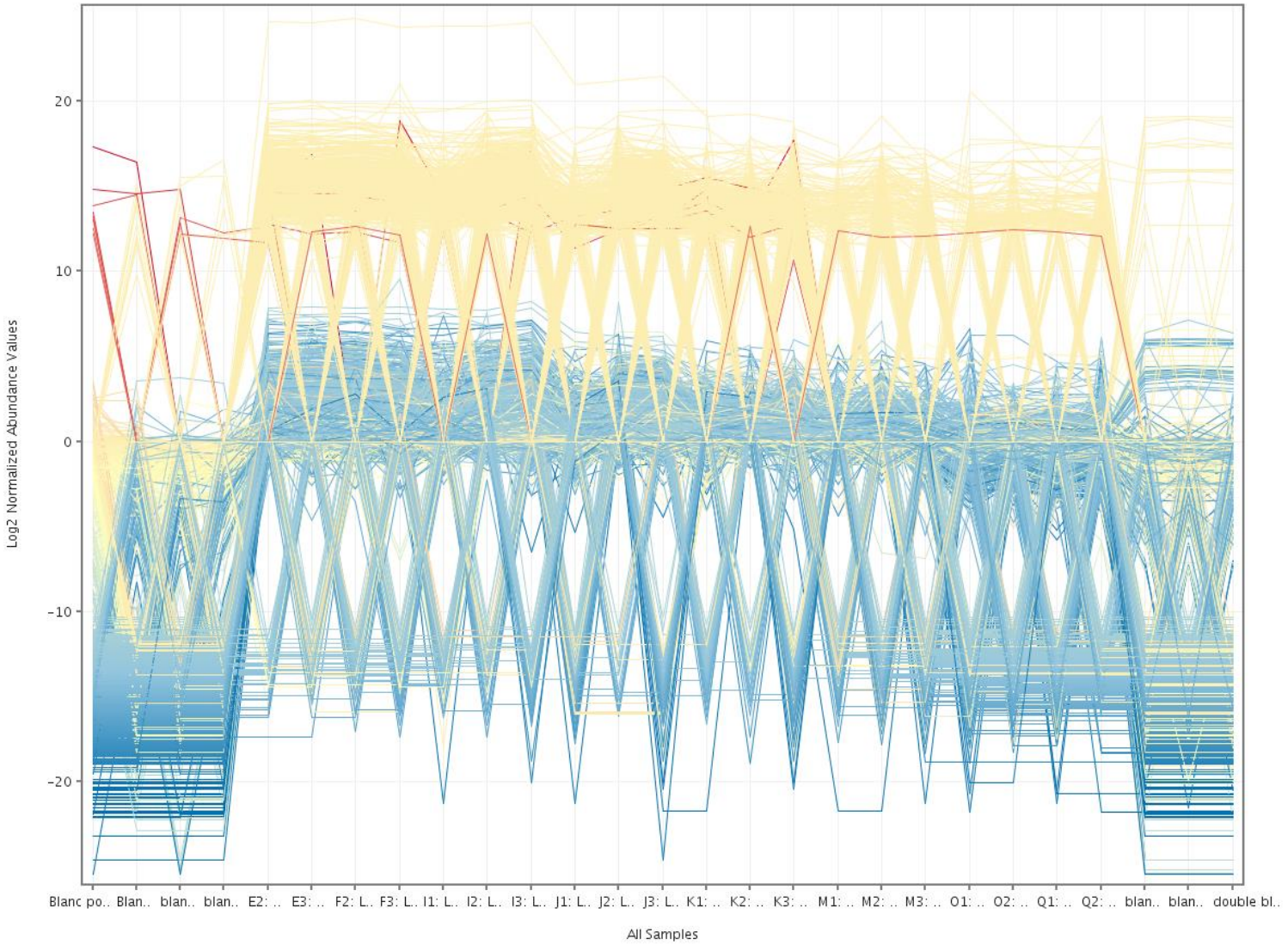
On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 3035 métabolites UP - FC ([J5] vs [Media])



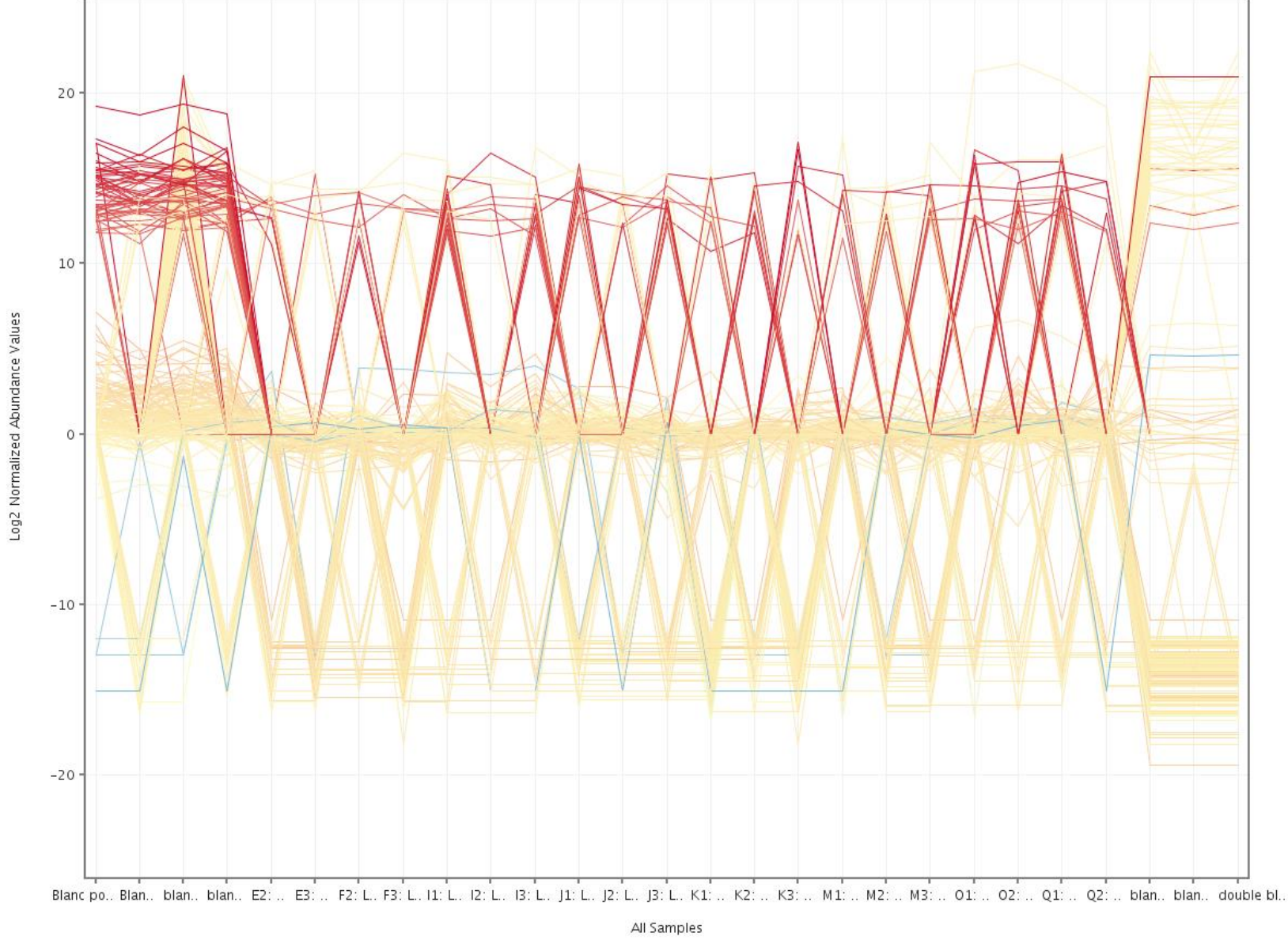
On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 259 métabolites DOWN - FC ([J5] vs [Media])



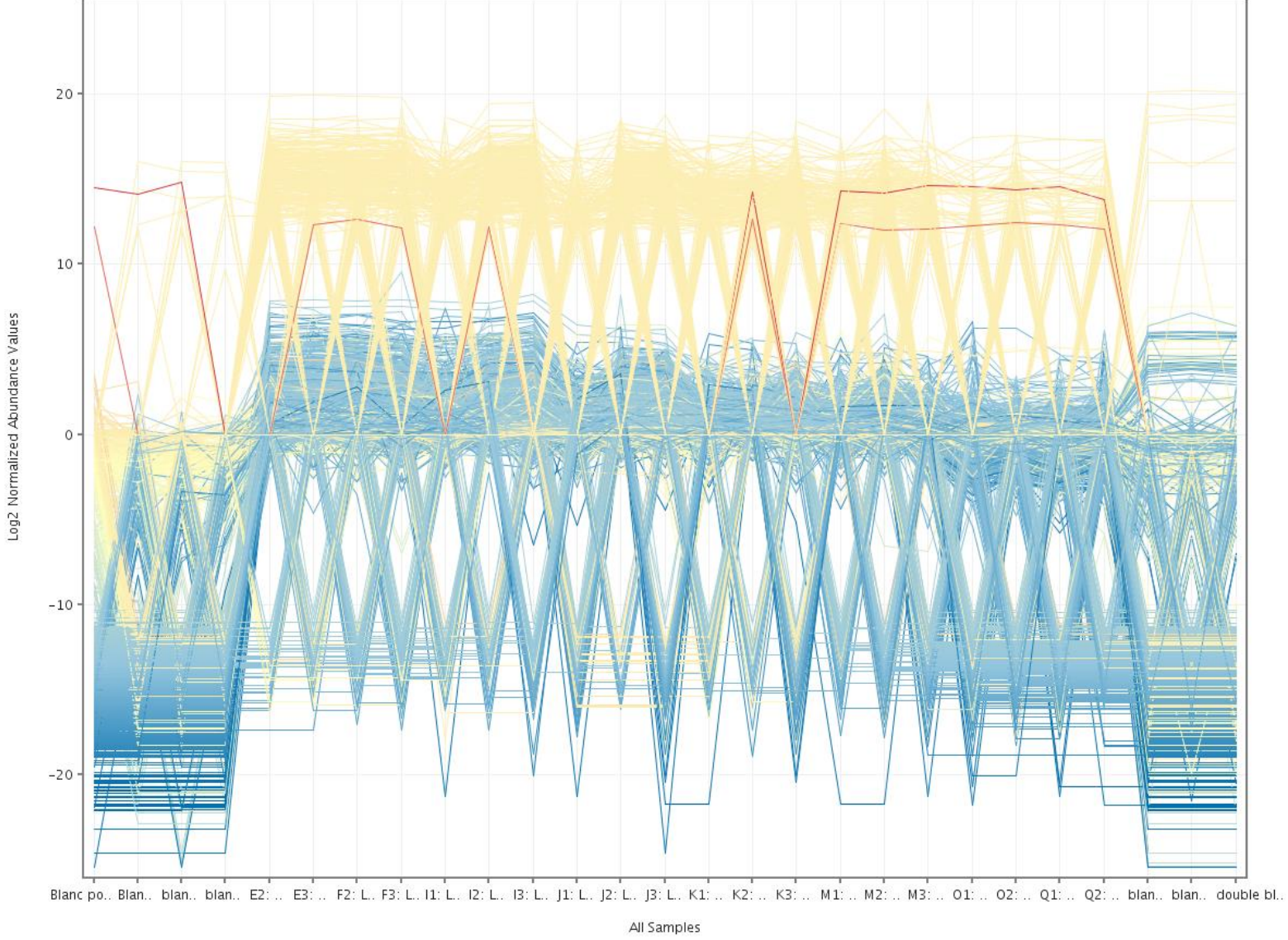
On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 2739 métabolites UP - FC ([J6] vs [Media])



On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 242 métabolites DOWN - FC ([J6] vs [Media])

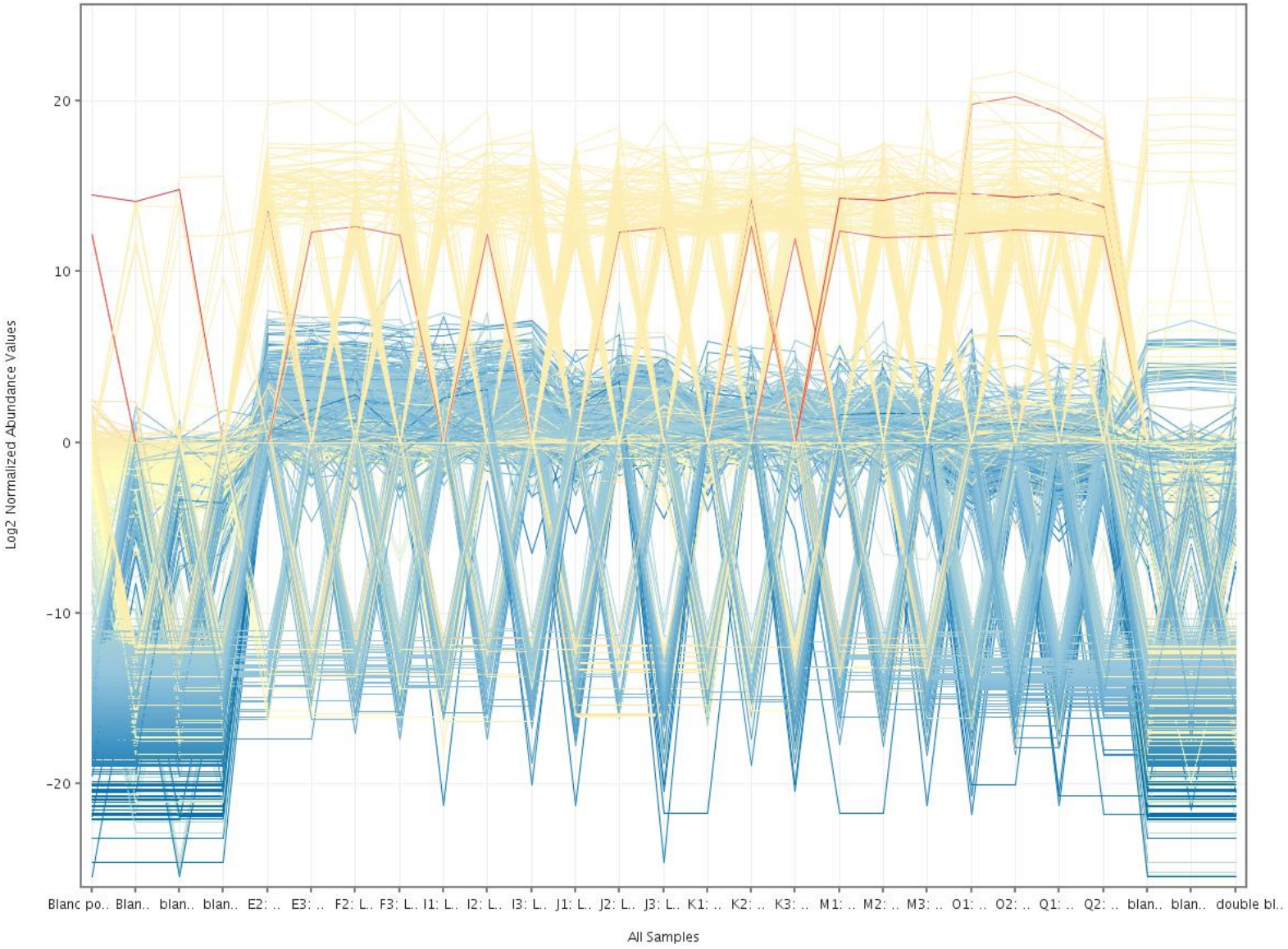


On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 2304 métabolites UP - FC ([J8] vs [Media])

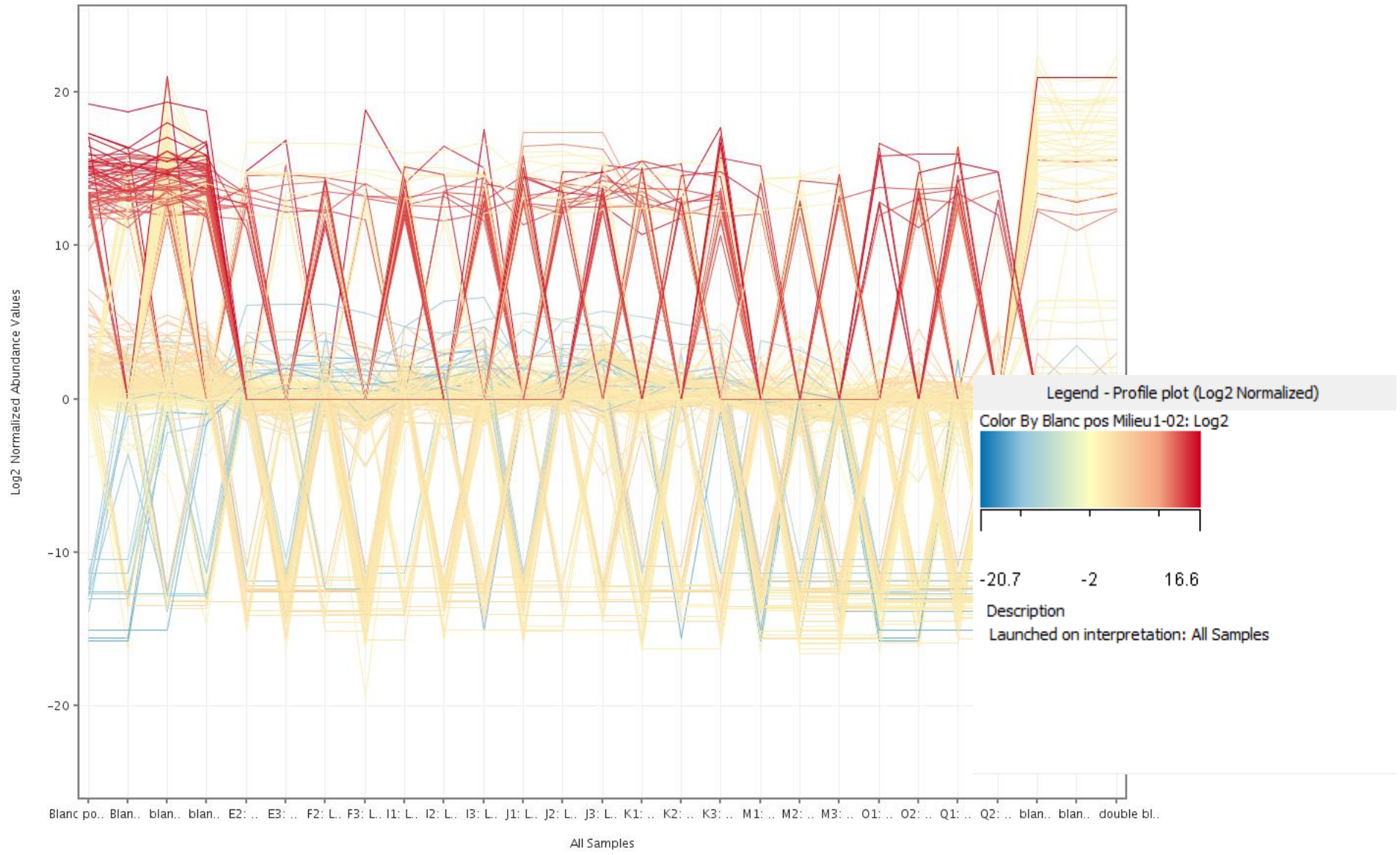
On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 389 métabolites DOWN - FC ([J8] vs [Media])



On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

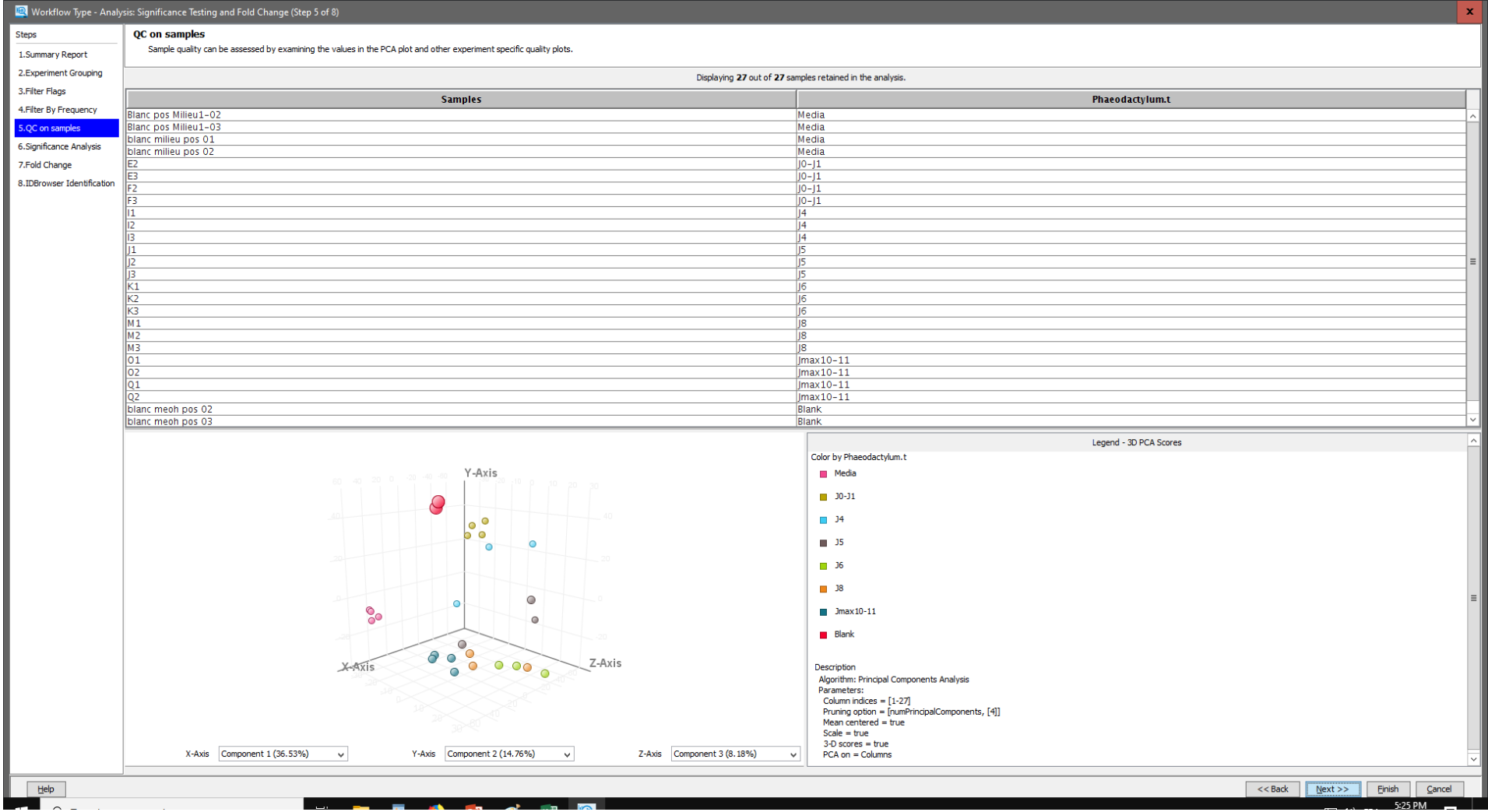
Ici les 1941 métabolites UP - FC ([Jmax10-11] vs [Media])



On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 329 métabolites DOWN - FC ([Jmax10-11] vs [Media])

SUITE III



Suite message Justine nvel analysis: significance testing & Fold Change

Workflow Type - Analysis: Significance Testing and Fold Change (Step 6 of 8)

Steps

1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification

Significance Analysis

Entities are filtered based on their p-values calculated from statistical analysis. To apply the new p-value cut-off, drag the "p-value cut-off" slider or input the new cut-off value in the text box. You will not be able to proceed to the next step if no entities pass the filter.

Displaying **4418** out of **5427** entities satisfying corrected p-value cut-off **0.05**.

Test Description

Selected Test:	Oneway ANOVA
p-value computation:	Asymptotic
Multiple Testing Correction:	Benjamini-Hochberg

Result Summary

	P all	P < 0.05	P < 0.02	P < 0.01	P < 0.005	P < 0.001
Corrected p-value	5427	4418	4090	3909	3731	3161
Expected by chance		220	81	39	18	3

Compound	p	p (Corr)
132.069@6.0720005	9.34E-05	1.80E-04
658.4239@20.819	4.83E-09	1.83E-08
829.5867@20.882998	2.67E-07	7.95E-07
610.1612@22.717997	5.87E-17	2.84E-16
790.4642@22.251005	1.08E-09	4.35E-09
390.2778@23.309	1.27E-03	2.01E-03
180.095@7.266001	6.90E-05	1.37E-04
337.1753@3.6430001	1.88E-10	7.79E-10
325.3714@17.399996	1.21E-08	4.38E-08
785.5088@22.243006	3.58E-09	1.38E-08
792.4799@23.026	4.37E-09	1.67E-08
558.1244@21.357996	2.32E-11	9.83E-11
658.4241@20.819	4.48E-09	1.71E-08
370.0943@21.366003	3.71E-19	2.04E-18
803.5699@20.553001	6.75E-28	1.29E-26
658.4239@21.679996	1.16E-09	4.67E-09
273.1808@1.7180002	3.02E-28	6.30E-27
520.2227@20.683996	2.95E-09	1.15E-08

p-value cut-off 0.05

Help | << Back | Next >> | Finish | Cancel

Workflow Type - Analysis: Significance Testing and Fold Change (Step 7 of 8)

Steps

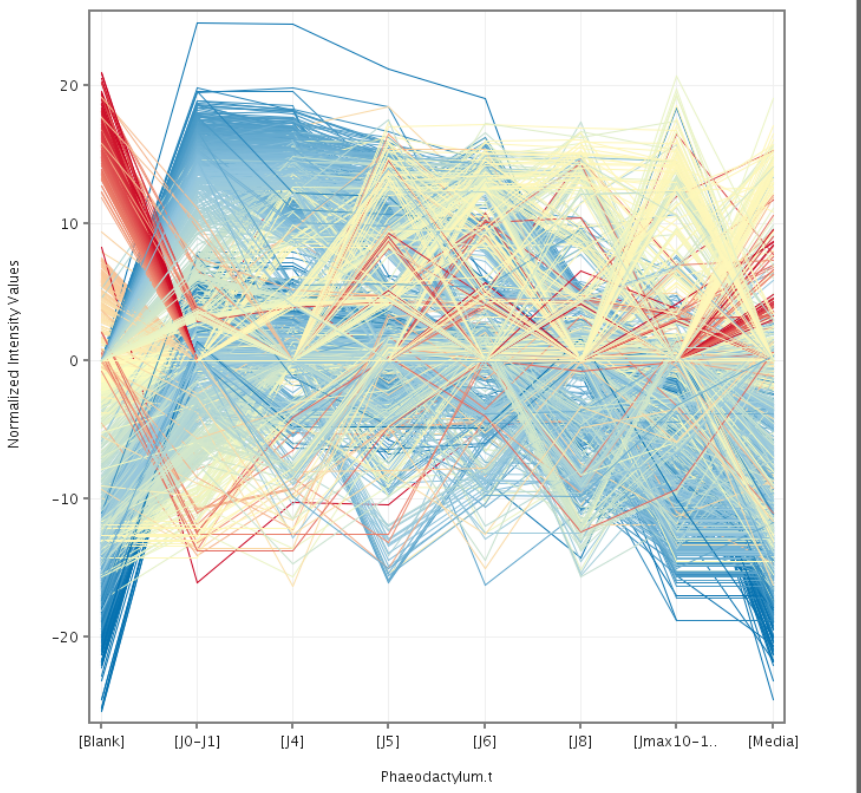
1.Summary Report
2.Experiment Grouping
3.Filter Flags
4.Filter By Frequency
5.QC on samples
6.Significance Analysis
7.Fold Change
8.IDBrowser Identification

Fold Change

Compounds that satisfy a fold change cut-off of 2.0 in at least one condition pair are displayed by default. To apply the new fold change cut-off, drag the "Fold change cut-off" slider or input the new cut-off value in the text box.

Displaying **4267** out of **4418** entities with fold change cut-off of **2.0** in **1** out of **7** condition pairs with **[J0-J1]** as the control condition.

Compound	FC ([Blank] ...	FC ([J4] vs [J...	FC ([J5] vs [...	FC ([J6] vs [J...	FC ([J8] vs [...	FC ([Jmax10...	FC ([Media] ...
132.069@6...	-38.69	3.16	2.30	1.65	2.41	-1.39	2.22
658.4239@...	-10468126...	-1.06	-1.50	-1.44	-2.65	-9.42	-30281.97
829.5867@...	-45866916...	1.01	-314.66	-1.12	-1.08	-2.24	-45866916...
610.1612@...	66.59	-1.03	-1.09	-1.00	-1.01	-1.01	1.10
790.4642@...	-60479592...	1.04	-1.09	-1.12	-1.41	-4.26	-33062.43
180.095@7...	-30559.09	51.72	30.22	27.67	25.79	13.65	28.27
337.1753@...	-45699616...	-1.27	-6.09	-27.41	-85.51	-269.21	-1011415.69
325.3714@...	-1.43	1.01	-1.01	1.40	-1.02	3.09	-1.77
785.5088@...	-38247340...	1.04	-1.14	-1.19	-1.54	-4.15	-16479.46
792.4799@...	-20595148...	1.25	-1.49	-2.84	-6.71	-26.24	-217777.34
558.1244@...	63.83	-1.20	-1.08	1.03	1.12	1.20	1.54
658.4241@...	-10475602...	-1.06	-1.50	-1.44	-2.66	-9.42	-31217.08
370.0943@...	84.63	1.04	1.04	1.05	-1.01	-1.05	1.02
803.5699@...	-13746878...	1.11	1.50	1.23	-1.42	-3.92	-13746878...
658.4239@...	-16126438...	-1.10	-1.92	-2.80	-7.56	-33.69	-1337734.50
273.1808@...	-26438788...	-1.11	-10.41	-49.20	-151.39	-394.49	-26438788...
520.2227@...	-561889.88	7.20	3.41	3.39	2.90	1.01	-3.64
678.5045@...	-1058.34	-1.13	-1.14	-1.06	1.14	-1.07	-1.60
330.3131@...	177.03	-1.04	-1.33	1.90	2.24	-1.02	-3.45
580.3922@...	-23518136...	-1.10	-1.94	-1.89	-5.04	-28.46	-311446.09
536.1418@...	51.63	1.01	1.02	1.05	1.01	-1.02	-1.02
658.4241@...	-14332426...	1.03	-1.48	-1.61	-3.57	-14.51	-22330.08
185.1061@...	-251500.00	2.51	3.36	2.47	2.39	3.76	47.12
750.5283@...	-12826288...	-6.93	-198.97	-1484.67	-74055.69	-2.08	-12826288...
418.3654@...	44.36	1.10	-1.33	1.48	1.27	-1.68	-4.21
287.1962@...	-17393188...	1.13	-4.24	-17.45	-60.50	-195.58	-17393188...
567.4708@...	14.23	1.05	-1.40	-1.05	-1.34	-2.03	-10.56
479.4185@...	24.69	1.05	-1.43	1.21	-1.02	-1.87	-4.42
300.2777@...	1.02	-1.08	1.14	-1.03	-1.04	51.04	-1.14
738.4331@...	-15640639...	-1.03	-2.47	-11.49	-61.34	-335.44	-1845224.38
611.4975@...	13.31	1.03	-1.38	-1.07	-1.39	-1.88	-11.90
374.3388@...	86.52	1.12	-1.45	1.68	1.79	-1.39	-3.15
257.0877@...	-4014.24	35.02	21.91	19.64	16.59	8.39	16.92
462.1234@...	45.55	-1.06	1.08	1.04	-1.16	-1.13	-1.10
655.5234@...	13.74	1.03	-1.34	-1.09	-1.36	-1.69	-12.62
354.0627@...	97.56	1.01	1.01	1.04	-1.02	-1.05	-1.02
787.5243@...	-13895176...	1.15	-1.43	-2.12	-4.04	-12.92	-1436767.62
606.4288@...	-16093809...	1.04	-1.51	-1.69	-3.17	-21.64	-1884433.38
755.568@2...	-3416135.25	1.39	1.38	1.39	-3.90	-101716.18	-3416135.25
790.4647@...	-60486468...	1.04	-1.09	-1.12	-1.41	-4.26	-466147.56
956.5491@...	-12150574...	1.05	-1.45	-2.01	-3.87	-12.43	-12150574...
612.1503@...	83.13	1.03	1.05	1.03	1.07	1.08	1.01



Fold change cut-off 2.0

Minimum no. of pairs 1

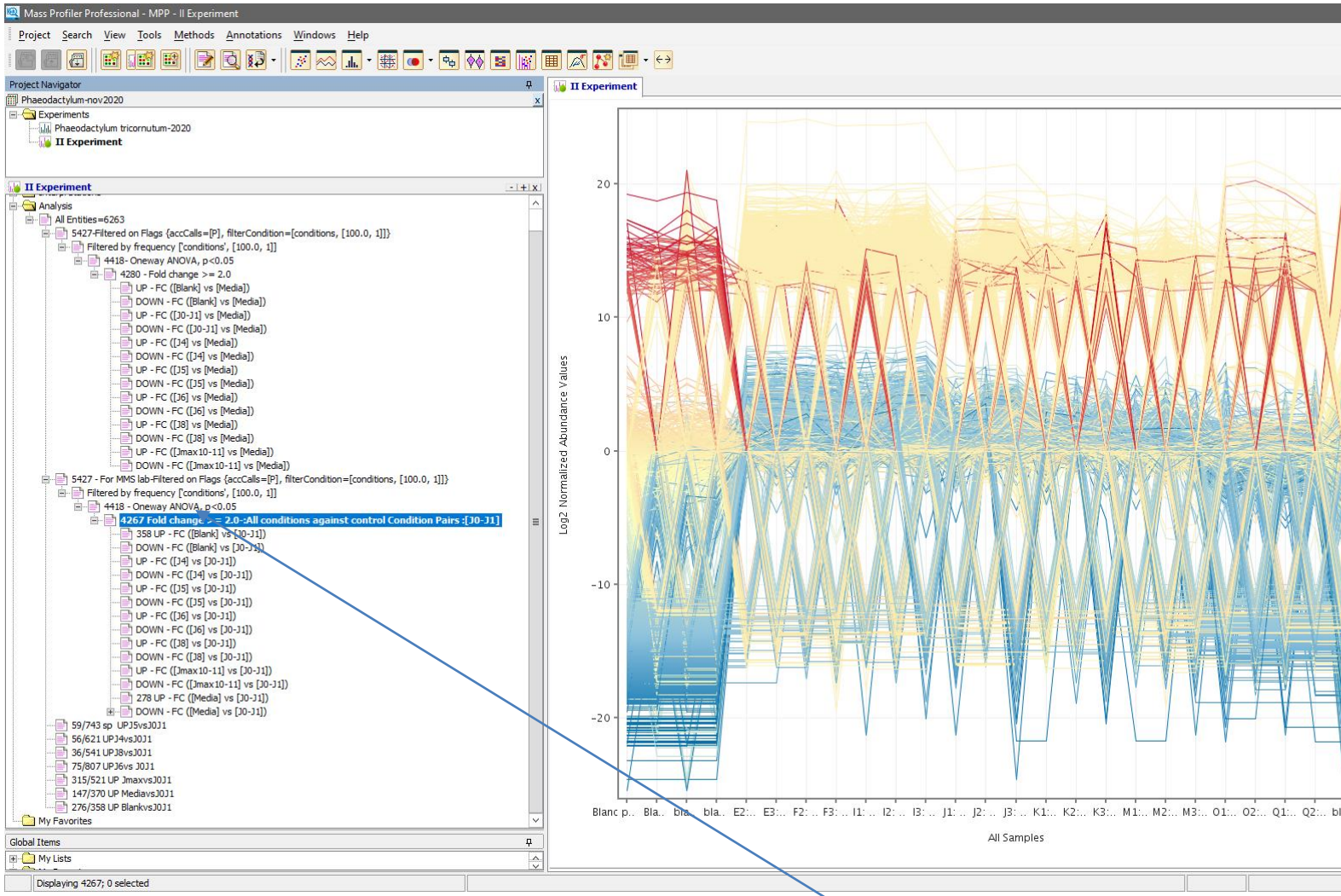
Control Group J0-J1

Help

<< Back | Next >> | Finish | Cancel

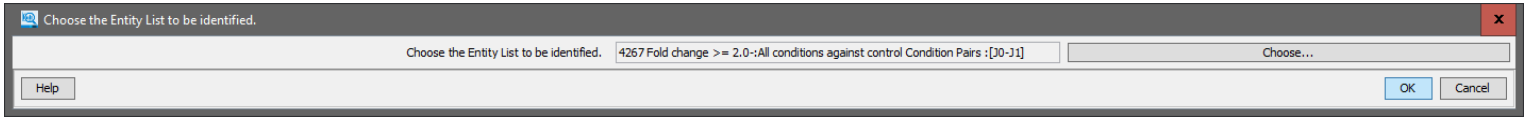
Changement de groupe et
J0-J1 sert de contrôle

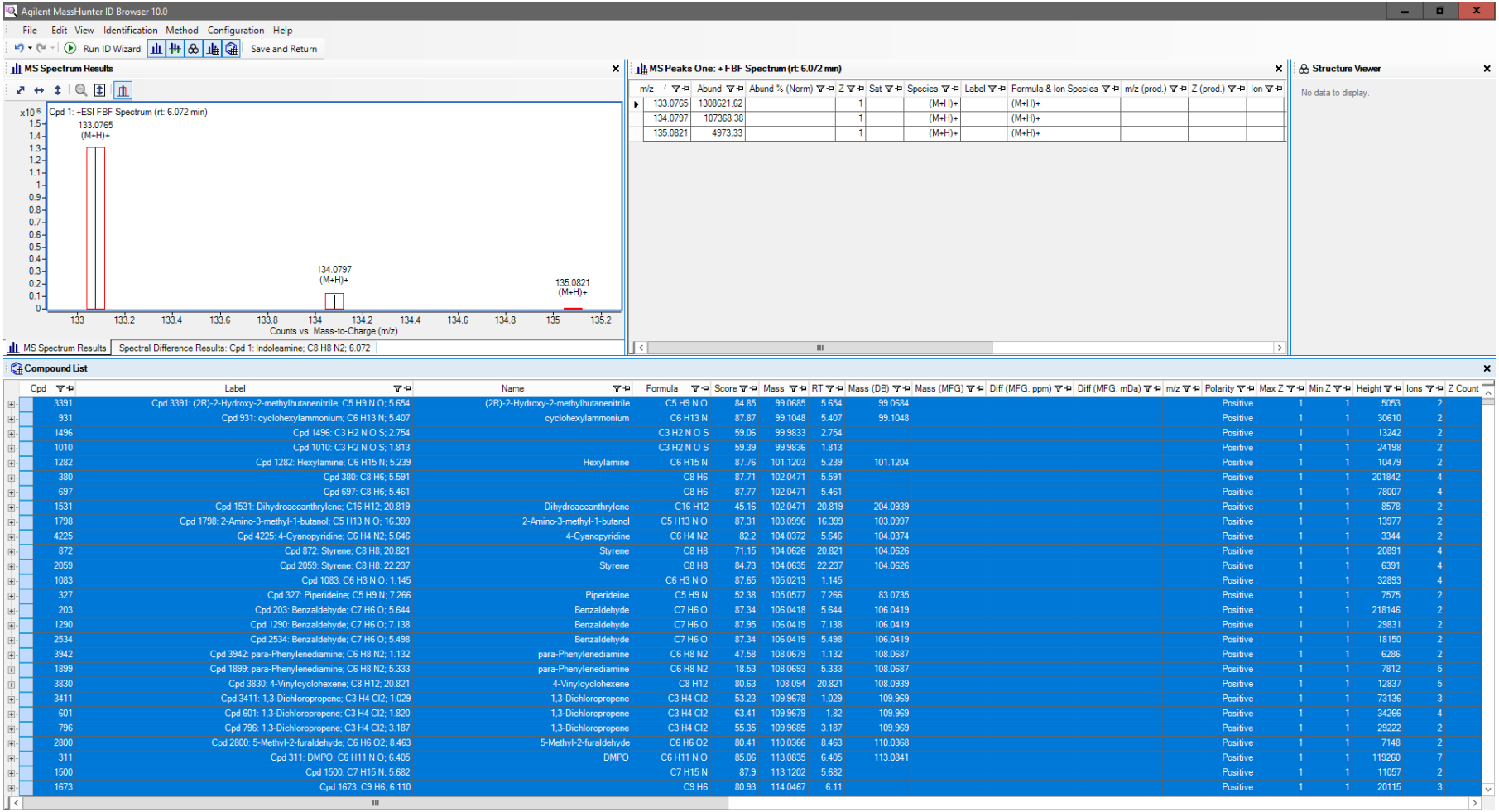
6- 2020 New Phaeodactylum MPP15v1.tar



Extraction du fichier : Phaeodactylum (without E1-F1) Foldchange sur J0-J1controle.xlsx 4267 entities comparés à la transcriptomique sur 115 composés communs (Results on115 composés MMS rev FM.xlsx)

Results interprétation by IDBrowser Identification





m/z	Abund	Abund % (Norm)	Z	Sat	Species	Label	Formula & Ion Species	m/z (prod.)	Z (prod.)	Ion
133.0765	1308621.62		1		(M+H)+		(M+H)+			
134.0797	107368.38		1		(M+H)+		(M+H)+			
135.0821	4973.33		1		(M+H)+		(M+H)+			

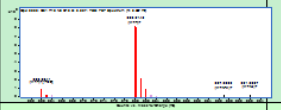
Cpd	Label	Name	Formula	Score	Mass	RT	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Diff (MFG, mDa)	m/z	Polarity	Max Z	Min Z	Height	Ions	Z Count
3391	Cpd 3391: (2R)-2-Hydroxy-2-methylbutanenitrile; C5 H9 N O; 5.654	(2R)-2-Hydroxy-2-methylbutanenitrile	C5 H9 N O	84.85	99.0685	5.654	99.0684					Positive	1	1	5053	2	
931	Cpd 931: cyclohexylammonium; C6 H13 N; 5.407	cyclohexylammonium	C6 H13 N	87.87	99.1048	5.407	99.1048					Positive	1	1	30610	2	
1496	Cpd 1496: C3 H2 N O S; 2.754		C3 H2 N O S	59.06	99.9833	2.754						Positive	1	1	13242	2	
1010	Cpd 1010: C3 H2 N O S; 1.813		C3 H2 N O S	59.39	99.9836	1.813						Positive	1	1	24198	2	
1282	Cpd 1282: Hexylamine; C6 H15 N; 5.239	Hexylamine	C6 H15 N	87.76	101.1203	5.239	101.1204					Positive	1	1	10479	2	
380	Cpd 380: C8 H6; 5.591		C8 H6	87.71	102.0471	5.591						Positive	1	1	201842	4	
697	Cpd 697: C8 H6; 5.461		C8 H6	87.77	102.0471	5.461						Positive	1	1	78007	4	
1531	Cpd 1531: Dihydroaceanthrylene; C16 H12; 20.819	Dihydroaceanthrylene	C16 H12	45.16	102.0471	20.819	204.0939					Positive	1	1	8578	2	
1798	Cpd 1798: 2-Amino-3-methyl-1-butanol; C5 H13 N O; 16.399	2-Amino-3-methyl-1-butanol	C5 H13 N O	87.31	103.0996	16.399	103.0997					Positive	1	1	13977	2	
4225	Cpd 4225: 4-Cyanopyridine; C6 H4 N2; 5.646	4-Cyanopyridine	C6 H4 N2	82.2	104.0372	5.646	104.0374					Positive	1	1	3344	2	
872	Cpd 872: Styrene; C8 H8; 20.821	Styrene	C8 H8	71.15	104.0626	20.821	104.0626					Positive	1	1	20891	4	
2059	Cpd 2059: Styrene; C8 H8; 22.237	Styrene	C8 H8	84.73	104.0635	22.237	104.0626					Positive	1	1	6391	4	
1083	Cpd 1083: C6 H3 N O; 1.145		C6 H3 N O	87.65	105.0213	1.145						Positive	1	1	32893	4	
327	Cpd 327: Piperideine; C5 H9 N; 7.266	Piperideine	C5 H9 N	52.38	105.0577	7.266	83.0735					Positive	1	1	7575	2	
203	Cpd 203: Benzaldehyde; C7 H6 O; 5.644	Benzaldehyde	C7 H6 O	87.34	106.0418	5.644	106.0419					Positive	1	1	218146	2	
1290	Cpd 1290: Benzaldehyde; C7 H6 O; 7.138	Benzaldehyde	C7 H6 O	87.95	106.0419	7.138	106.0419					Positive	1	1	29831	2	
2534	Cpd 2534: Benzaldehyde; C7 H6 O; 5.498	Benzaldehyde	C7 H6 O	87.34	106.0419	5.498	106.0419					Positive	1	1	18150	2	
3942	Cpd 3942: para-Phenylenediamine; C6 H8 N2; 1.132	para-Phenylenediamine	C6 H8 N2	47.58	108.0679	1.132	108.0687					Positive	1	1	6286	2	
1899	Cpd 1899: para-Phenylenediamine; C6 H8 N2; 5.333	para-Phenylenediamine	C6 H8 N2	18.53	108.0693	5.333	108.0687					Positive	1	1	7812	5	
3830	Cpd 3830: 4-Vinylcyclohexene; C8 H12; 20.821	4-Vinylcyclohexene	C8 H12	80.63	108.094	20.821	108.0939					Positive	1	1	12837	5	
3411	Cpd 3411: 1,3-Dichloropropene; C3 H4 Cl2; 1.029	1,3-Dichloropropene	C3 H4 Cl2	53.23	109.9678	1.029	109.969					Positive	1	1	73136	3	
601	Cpd 601: 1,3-Dichloropropene; C3 H4 Cl2; 1.820	1,3-Dichloropropene	C3 H4 Cl2	63.41	109.9679	1.82	109.969					Positive	1	1	34266	4	
796	Cpd 796: 1,3-Dichloropropene; C3 H4 Cl2; 3.187	1,3-Dichloropropene	C3 H4 Cl2	55.35	109.9685	3.187	109.969					Positive	1	1	29222	2	
2800	Cpd 2800: 5-Methyl-2-furaldehyde; C6 H6 O2; 8.463	5-Methyl-2-furaldehyde	C6 H6 O2	80.41	110.0366	8.463	110.0368					Positive	1	1	7148	2	
311	Cpd 311: DMPO; C6 H11 N O; 6.405	DMPO	C6 H11 N O	85.06	113.0835	6.405	113.0841					Positive	1	1	119260	7	
1500	Cpd 1500: C7 H15 N; 5.682		C7 H15 N	87.9	113.1202	5.682						Positive	1	1	11057	2	
1673	Cpd 1673: C9 H6; 6.110		C9 H6	80.93	114.0467	6.11						Positive	1	1	20115	3	

Pour compléter l'identification des composés commun à la transcriptomique

Results on115 composés MMS rev FM.xlsx - Excel

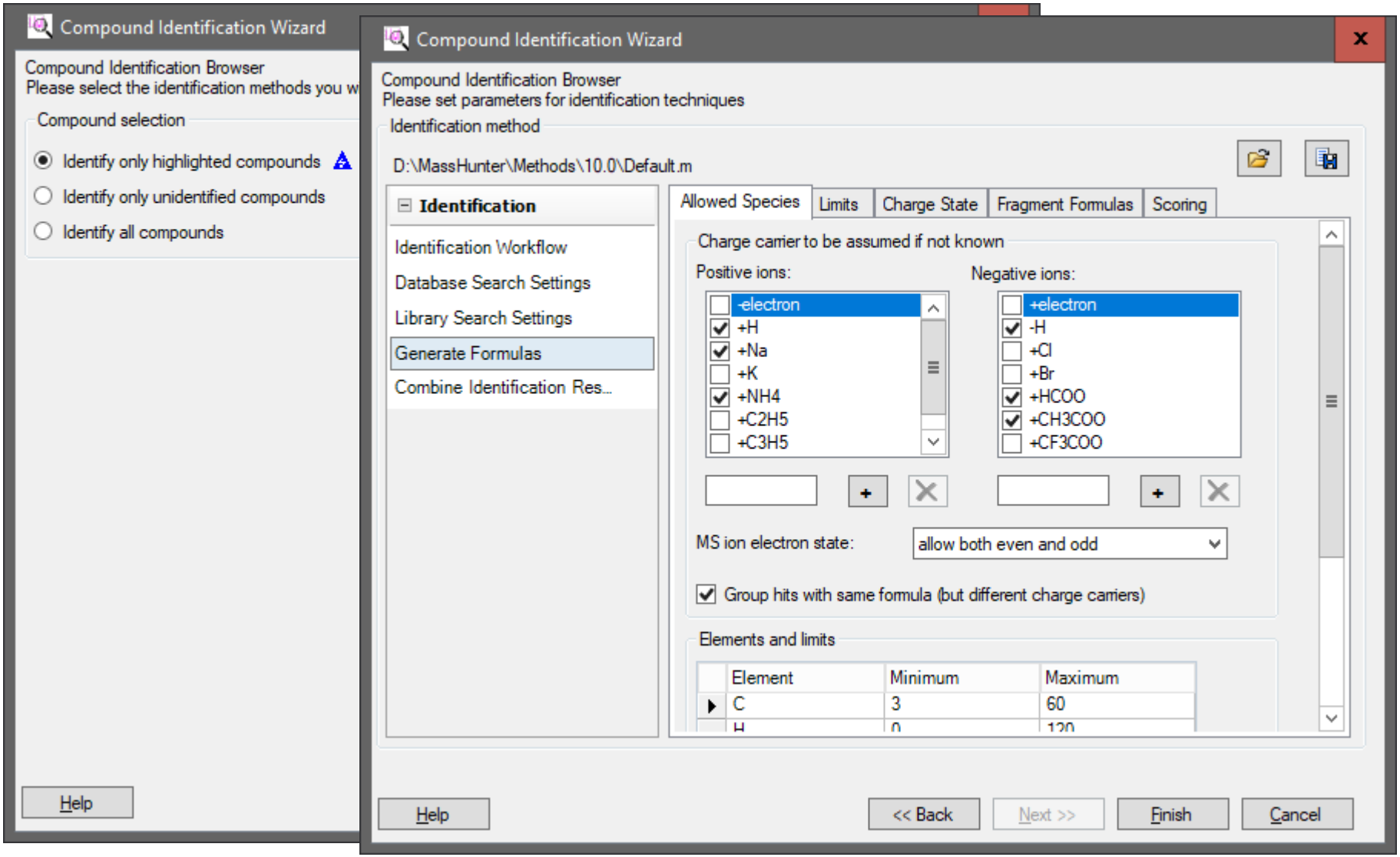
FICHIER ACCUEIL INSERTION MISE EN PAGE FORMULES DONNÉES RÉVISION AFFICHAGE MASSHUNTER REPORTING Connexion

L53

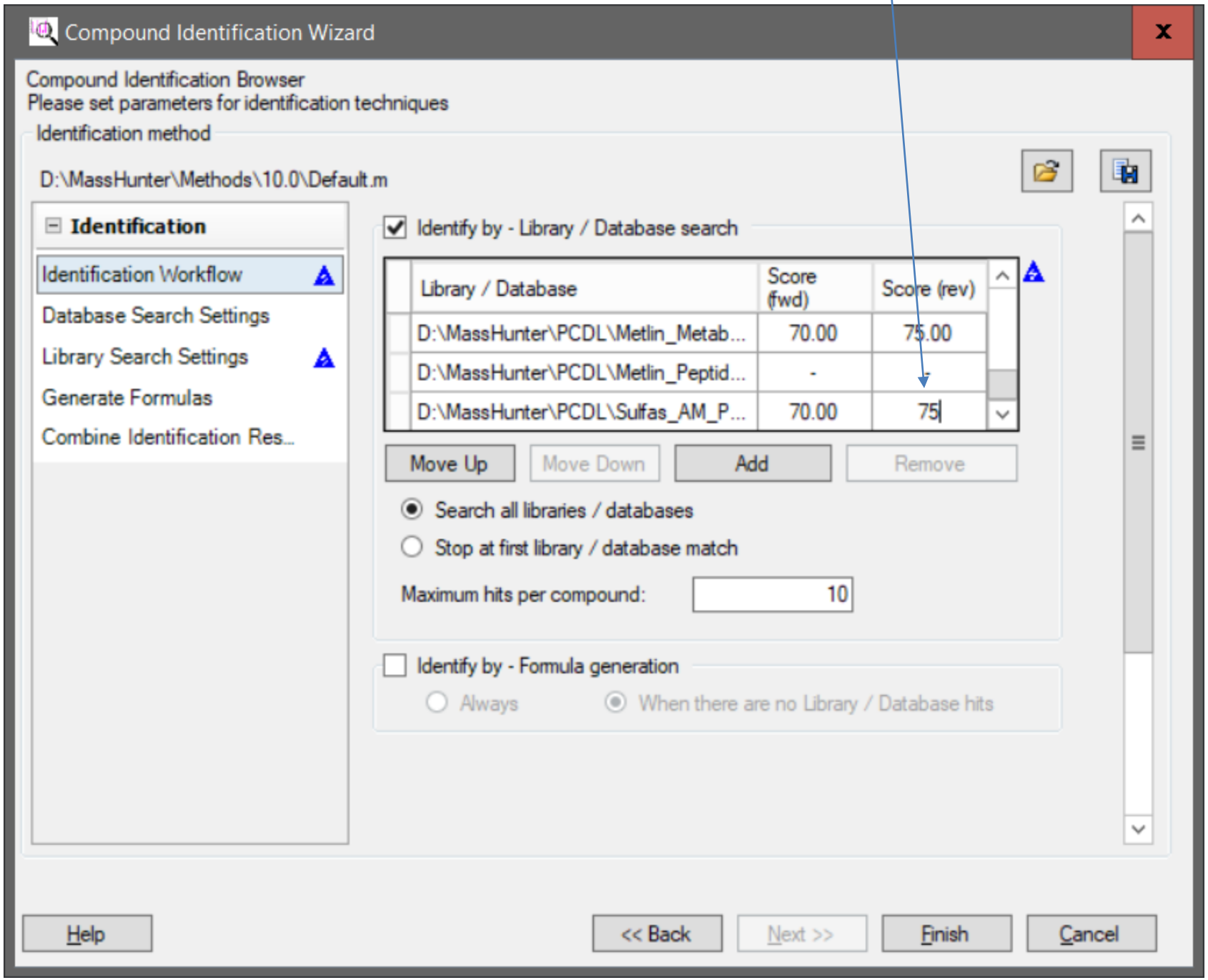
	A	B	C	D	E	F	G	H	I	J
1	Compound	Rt	R-square	P-value	Name	Formula	Score	Know/unknow		Compound,R-square,P-value
2	102.0471	5.5910015	0.999622924	3.11E-06		C8H6	87.71	unknow		102.0471@5.5910015,0.999622924,3.11E-06
3	118.0417	3.7160008	0.999478153	5.06E-06		C8H6O	87.23			118.0417@3.7160008,0.999478153,5.06E-06
4	126.1046	20.812004	0.983597726	0.00089597	4-Vinylcyclohexene	C8 H12	87.55			126.1046@20.812004,0.983597726,0.0008
5	129.0793	1.7859998	0.998738037	1.90E-05	minocyclopentane-1-carboxylic acid	C6 H11 N O2	78.81			129.0793@1.7859998,0.998738037,1.9
6	132.0690	6.0720005	0.957400597	0.0037804	Indoleamine	C8 H8N2	97.72			132.069@6.0720005,0.957400597,0.00
7	137.0854	5.5899982	0.996877349	7.41E-05	4-Amino-3,5-xylenol	C8 H11 N O	47.31			137.0854@5.5899982,0.996877349,7.4
8	143.0738	6.111	0.998183761	3.29E-05	1-Naphthylamine	C10H9N	87.57			143.0738@6.111,0.998183761,3.2
9	164.0483	3.7160008	0.998948801	1.45E-05	Phenylpyruvic acid	C9 H8 O3	83.11			164.0483@3.7160008,0.998948801,1.4
10	164.0632	20.819	0.985238893	0.00076454	Phenylheptatriyne	C13 H8	67.81			164.0632@20.819,0.985238893,0.0007
11	165.0799	5.5899982	0.998985171	1.37E-05	-Pyridyl)-2-hydroxytetrahydrofuran	C9 H11 N O2	96.03			165.0799@5.5899982,0.998985171,1.3
12	187.0640	6.11	0.999721181	1.98E-06	Quinacetol OU 3-amino-2-naphthoic acid OU Indoleacrylic acid	C11 H9 N O2	94.98			187.064@6.11,0.999721181,1.98E-06

Feuil1

PRÊT 100%



Il faudrait recommencer l'analyse sur l'ensemble des base en spécifiant le nb de C, H, N, etc de telle manière que l'on n'ait pas de N14 (max5) et augmenter le nb de C pour ne pas etre sous la lim… bref de manière à améliorer le score des 115 composés à identifier à faire: 04/02/2021


Compound Identification Wizard
Compound Identification Browser
Please set parameters for identification techniques
Identification method
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Identification
Identification Workflow
Database Search Settings
Library Search Settings
Generate Formulas
Combine Identification Res...
Identify by - Library / Database search
Library / Database
Score (fwd)
Score (rev)
D:\MassHunter\PCDL\Metlin_Metab...
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75.00
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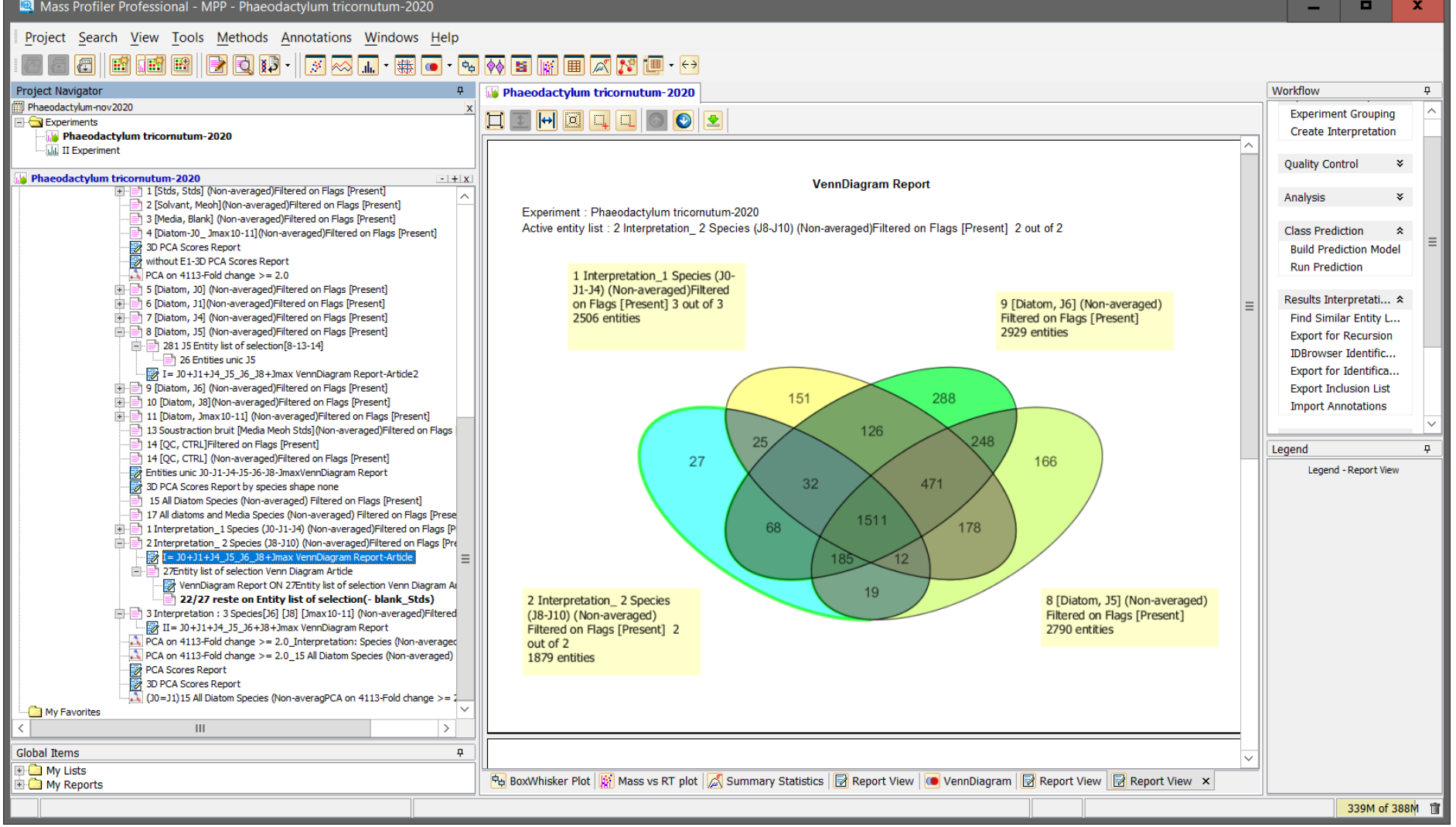
-
-
D:\MassHunter\PCDL\Sulfas_AM_P...
70.00
75
Move Up
Move Down
Add
Remove
Search all libraries / databases
Stop at first library / database match
Maximum hits per compound:
10
Identify by - Formula generation
Always
When there are no Library / Database hits
Help
<< Back
Next >>
Finish
Cancel



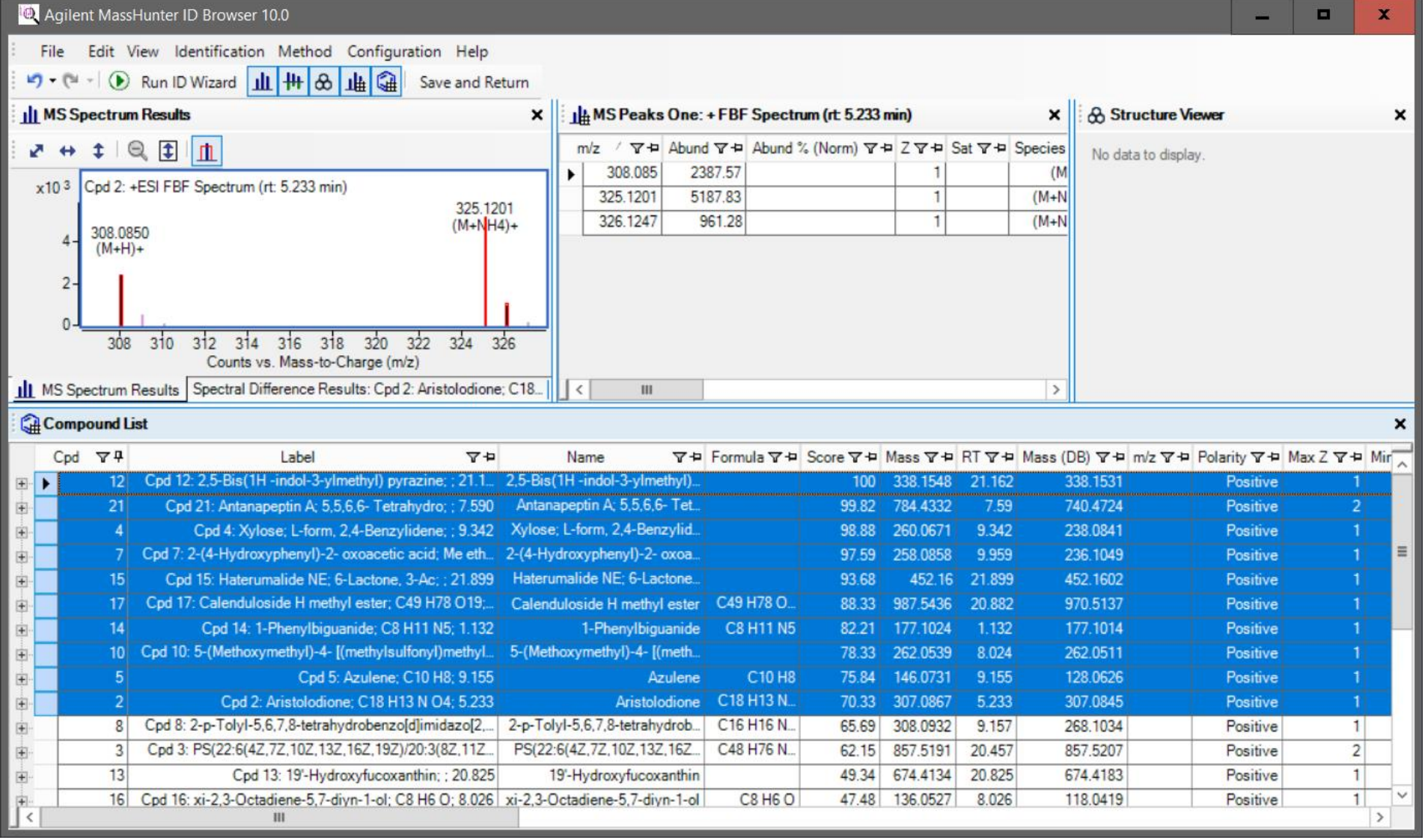
Comparaison Analyse 1:

Hy1= J0+JJ+J4; - J5; - J6 et Hy2= J8+Jmax

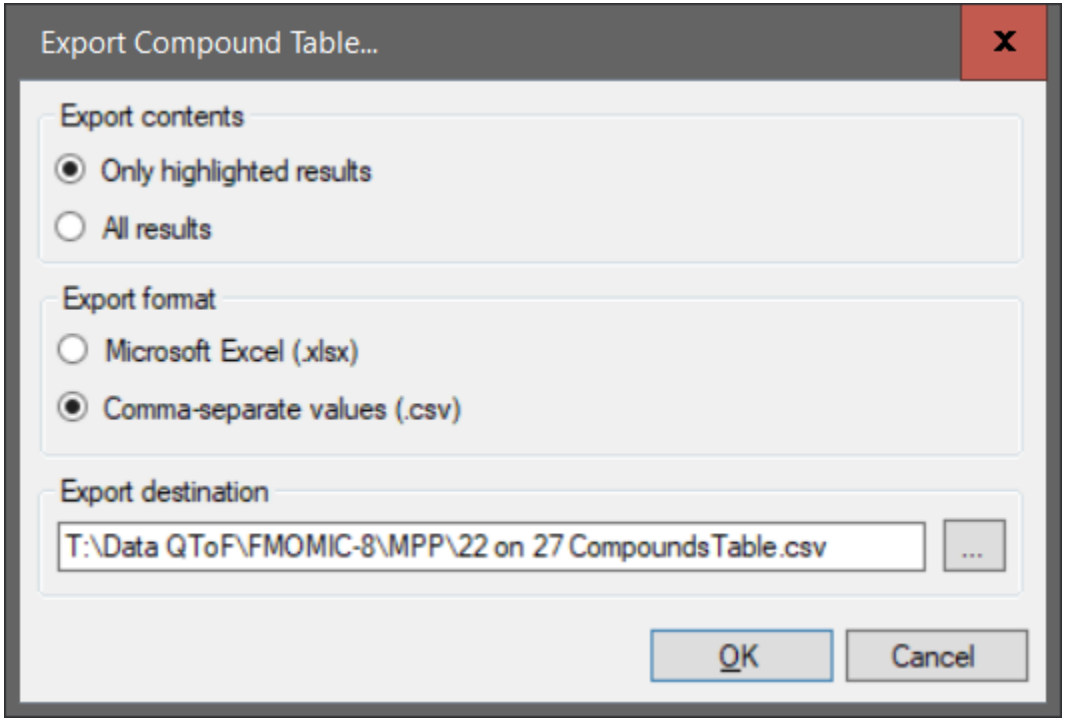
Avec Hy1 100% of the values in any 3 out of 3 conditions have acceptable values

Et Hy2 2 out of 2

puis Results interprétation by IDBrowser Identification sur le compartiment 27 (Demandé par Justine)



File-Export compound table



Ouvrir ce fichier. Csv dans Excel (séparateur: point-virgule)

Recherche du phosphoenolpyruvate; Phosphoenolpyruvic acid; 138-08-9; 2-Propenoic acid, 2-(phosphonooxy)-; 2-(phosphonooxy)prop-2-enoic acid; Phosphopyruvic acid; 2-Phosphonooxyprop-2-enoic acid; PEP; ...

Compound CID: 1005

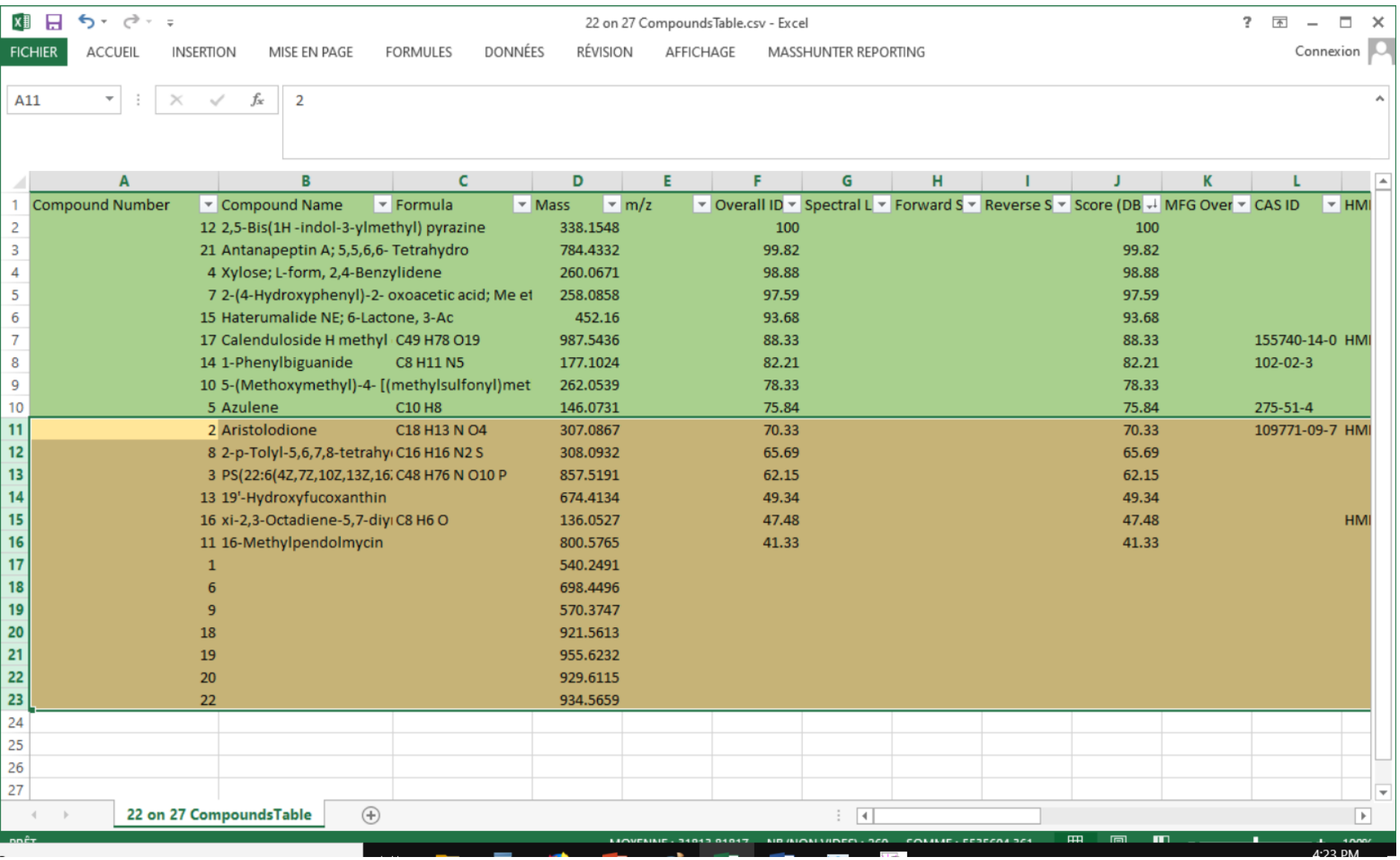
MF: $C_3H_5O_6P$

MW: 168.04g/mol

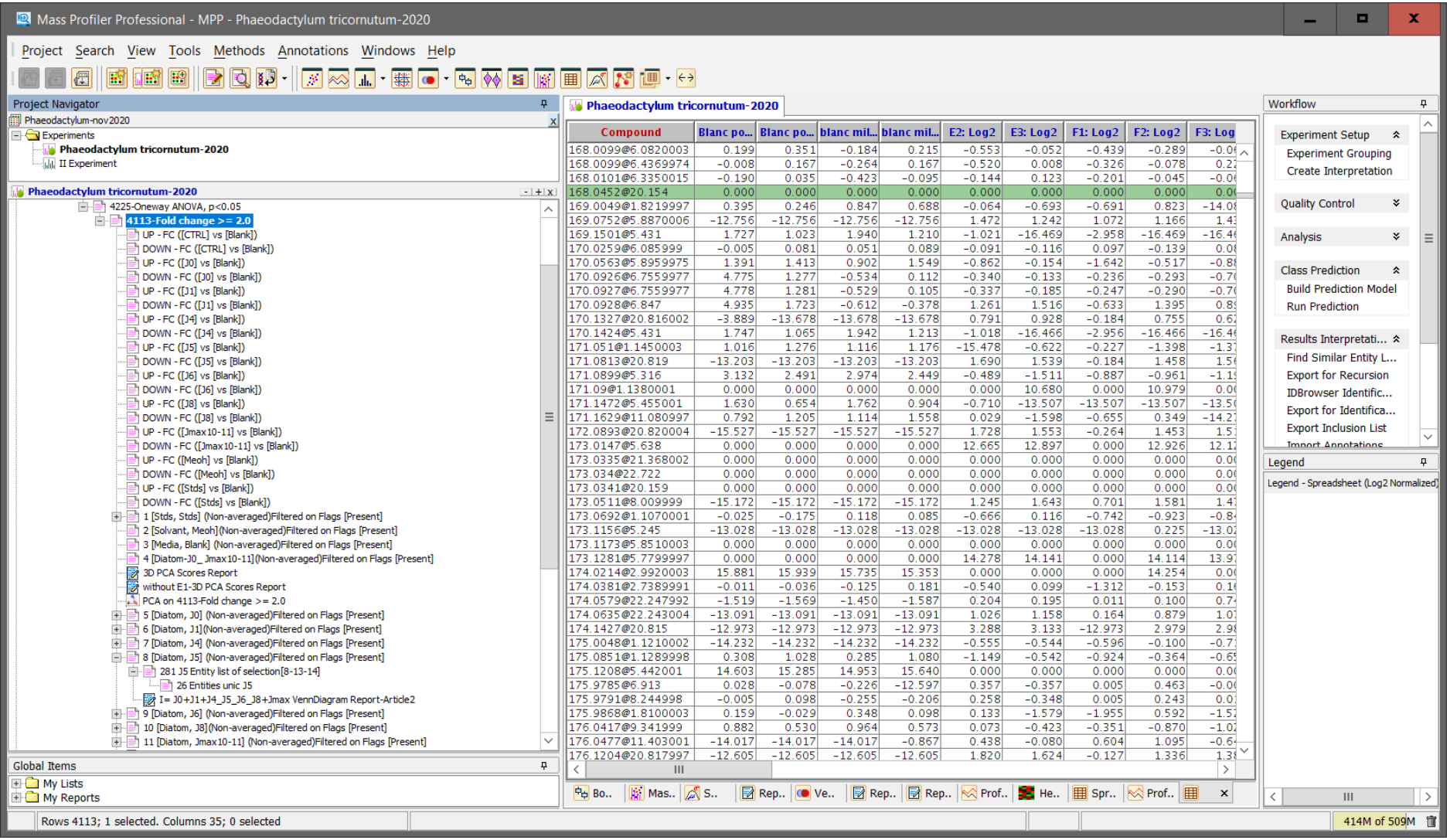
InChIKey: DTBNBXWJWCWCIK-UHFFFAOYSA-N

IUPAC Name: 2-phosphonooxyprop-2-enoic acid

Create Date: 2004-09-16



Compound Number	Compound Name	Formula	Mass	m/z	Overall ID	Spectral L	Forward S	Reverse S	Score (DB	MFG Over	CAS ID	HMI
12	2,5-Bis(1H -indol-3-ylmethyl) pyrazine		338.1548		100				100			
21	Antanapeptin A; 5,5,6,6- Tetrahydro		784.4332		99.82				99.82			
4	Xylose; L-form, 2,4-Benzylidene		260.0671		98.88				98.88			
7	2-(4-Hydroxyphenyl)-2- oxoacetic acid; Me et		258.0858		97.59				97.59			
15	Haterumalide NE; 6-Lactone, 3-Ac		452.16		93.68				93.68			
17	Calenduloside H methyl	C49 H78 O19	987.5436		88.33				88.33		155740-14-0	HMI
14	1-Phenylbiguanide	C8 H11 N5	177.1024		82.21				82.21		102-02-3	
10	5-(Methoxymethyl)-4- [(methylsulfonyl)met		262.0539		78.33				78.33			
5	Azulene	C10 H8	146.0731		75.84				75.84		275-51-4	
2	Aristolodione	C18 H13 N O4	307.0867		70.33				70.33		109771-09-7	HMI
8	2-p-Tolyl-5,6,7,8-tetrahy	C16 H16 N2 S	308.0932		65.69				65.69			
3	PS(22:6(4Z,7Z,10Z,13Z,16	C48 H76 N O10 P	857.5191		62.15				62.15			
13	19'-Hydroxyfucoxanthin		674.4134		49.34				49.34			
16	xi-2,3-Octadiene-5,7-diy	C8 H6 O	136.0527		47.48				47.48			HMI
11	16-Methylpendolmycin		800.5765		41.33				41.33			
1			540.2491									
6			698.4496									
9			570.3747									
18			921.5613									
19			955.6232									
20			929.6115									
22			934.5659									



Recherche du [phosphoenolpyruvate; Phosphoenolpyruvic acid; 138-08-9; 2-Propenoic acid, 2-(phosphonooxy)-; 2-(phosphonooxy)prop-2-enoic acid; Phosphopyruvic acid; 2-Phosphonooxyprop-2-enoic acid; PEP; ...]

Compound CID: [1005] - MF: $C_3H_5O_6P$ MW: 168.04g/mol

Bizarrement ce composé est à zero partout… (en fait uniquement dans Blancs et stds…cf Profinder)

FIN