Compounds in Orange- Increased Concentration
Compounds in Green - cluster 2
Compounds in Blue - cluster 3

15	D-(+)-Turanose, octakis(trimethylsilyl) ether
42	Glycerol monostearate, 2TMS derivative
39	1-Monopalmitin, 2TMS derivative
6	Lactic Acid, 2TMS derivative
11	Benzoic Acid, TMS derivative
27	Diethylene glycol, 2TMS derivative
13	Propane, 2-methyl-1,2-bis(trimethylsiloxy)-
29	1,3-Propanediol, 2TMS derivative
4	Nonane, 5-(2-methylpropyl)-
12	3-.alpha.-Mannobiose, octakis(trimethylsilyl) ether (isomer 2)
41	Dodecane, 4,6-dimethyl-
32	3-Ethyl-3-methylheptane
33	Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-
28	Sucrose, 8TMS derivative
36	Undecane, 5-methyl-
48	Thymol-.beta.-d-glucopyranoside, tetrakis(O-trimethylsilyl)-
57	N-(tert-butyldimethylsilyl)-2,2,2-trifluoro-N-methylacetamide

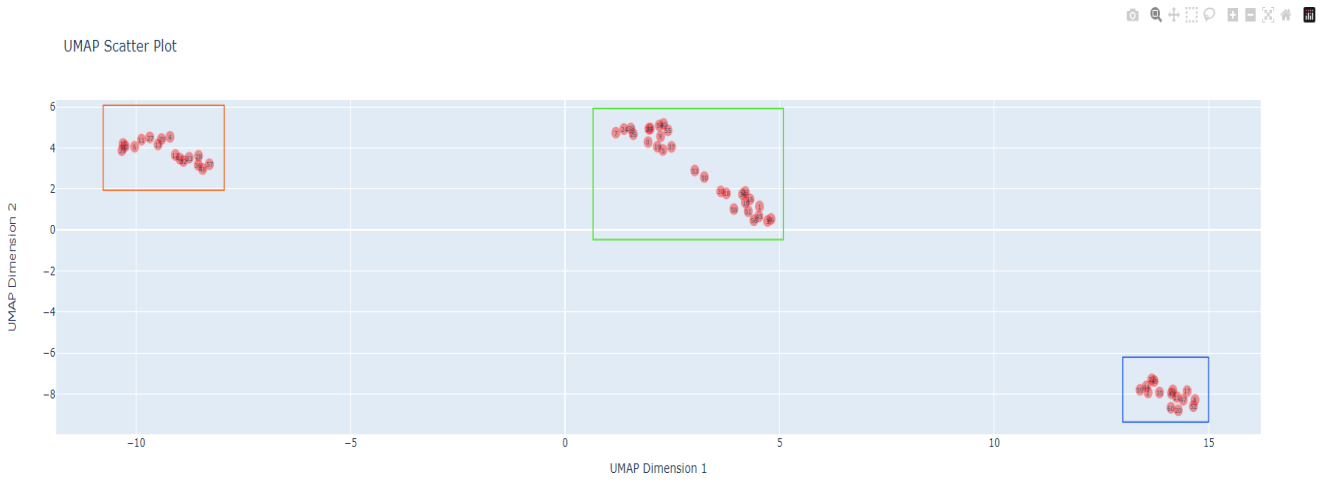
7	Ethyl .alpha.-D-glucopyranoside, 4TMS derivative
24	Heptasiloxane, hexadecamethyl-
38	1-Octanol, 2,2-dimethyl-
26	.beta.-D-Lactose, (isomer 1), 8TMS derivative
0	Heptadecane, 8-methyl-
25	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-, O-methyloxime
14	Glycerol, 3TMS derivative
54	1,4-Butanediol, 2TMS derivative
40	.beta.-Gentiobiose, octakis(trimethylsilyl) ether, methyloxime (isomer 1)
9	D-Fructose, 3-O-[2,3,4,6-tetrakis-O-(trimethylsilyl)-.alpha.-D-glucopyranosyl]-1,4,5,6-tetrakis-O-(trimethylsilyl)-
55	Dibutyl phthalate
19	Ethylene glycol, 2TMS derivative
5	D-(+)-Cellobiose, (isomer 1), 8TMS derivative
37	Eicosane
53	L-Threitol, 4TMS derivative
50	Octane, 2-methyl-
30	Adonitol, 5TMS derivative
18	Triethylene glycol, 2TMS derivative

58	Erythrono-1,4-lactone, (E)-, 2TMS derivative
34	Xylitol, 5TMS derivative

23	d-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxyme, (1Z)-
10	Palmitic Acid, TMS derivative
16	1,5-Anhydroglucitol, 4TMS derivative
51	D-(-)-Rhamnose, tetrakis(trimethylsilyl) ether, methyloxime (syn)
1	Melibiose, octakis(trimethylsilyl)-
45	Lactose, 8TMS derivative
56	Maltose, octakis(trimethylsilyl) ether, methyloxime (isomer 1)
3	D-(+)-Talose, pentakis(trimethylsilyl) ether, methyloxime (syn)
46	Glucose, 5TMS derivative

59	Cyclononasiloxane, octadecamethyl-
44	.alpha.-L-Galactofuranose, 6-deoxy-1,2,3,5-tetrakis-O-(trimethylsilyl)-
2	3-.alpha.-Mannobiose, octakis(trimethylsilyl) ether, methyloxime (isomer 1)D-Glucitol, 6TMS derivative
22	D-Glucitol, 6TMS derivative

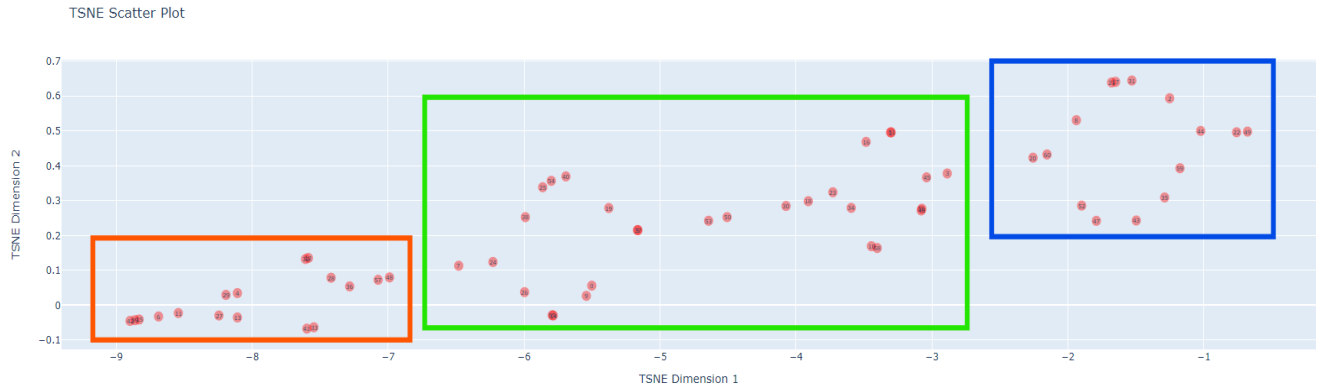
49	D-Arabinose, tetrakis(trimethylsilyl) ether, ethyloxime (isomer 2)
35	1,2,3,4,5,6-Hexa-O-trimethelsilyl-myo-inositol
60	L-(+)-Erythrulose, tris(trimethylsilyl) ether, trimethylsilyloxime (isomer 1)
43	L-Rhamnose, 4TMS derivative
31	D-Allose, oxime (isomer 1), 6TMS derivative
21	L-(+)-Erythrulose, tris(trimethylsilyl) ether, ethyloxime (isomer 1)
20	D-Galactose, 6-deoxy-2,3,4,5-tetrakis-O-(trimethylsilyl)-, O-methyloxime
47	Galactinol, nonakis(trimethylsilyl) ether
17	Dulcitol, 6TMS derivative
52	Levoglucosan, 3TMS derivative
8	Hexadecane, 1-iodo-

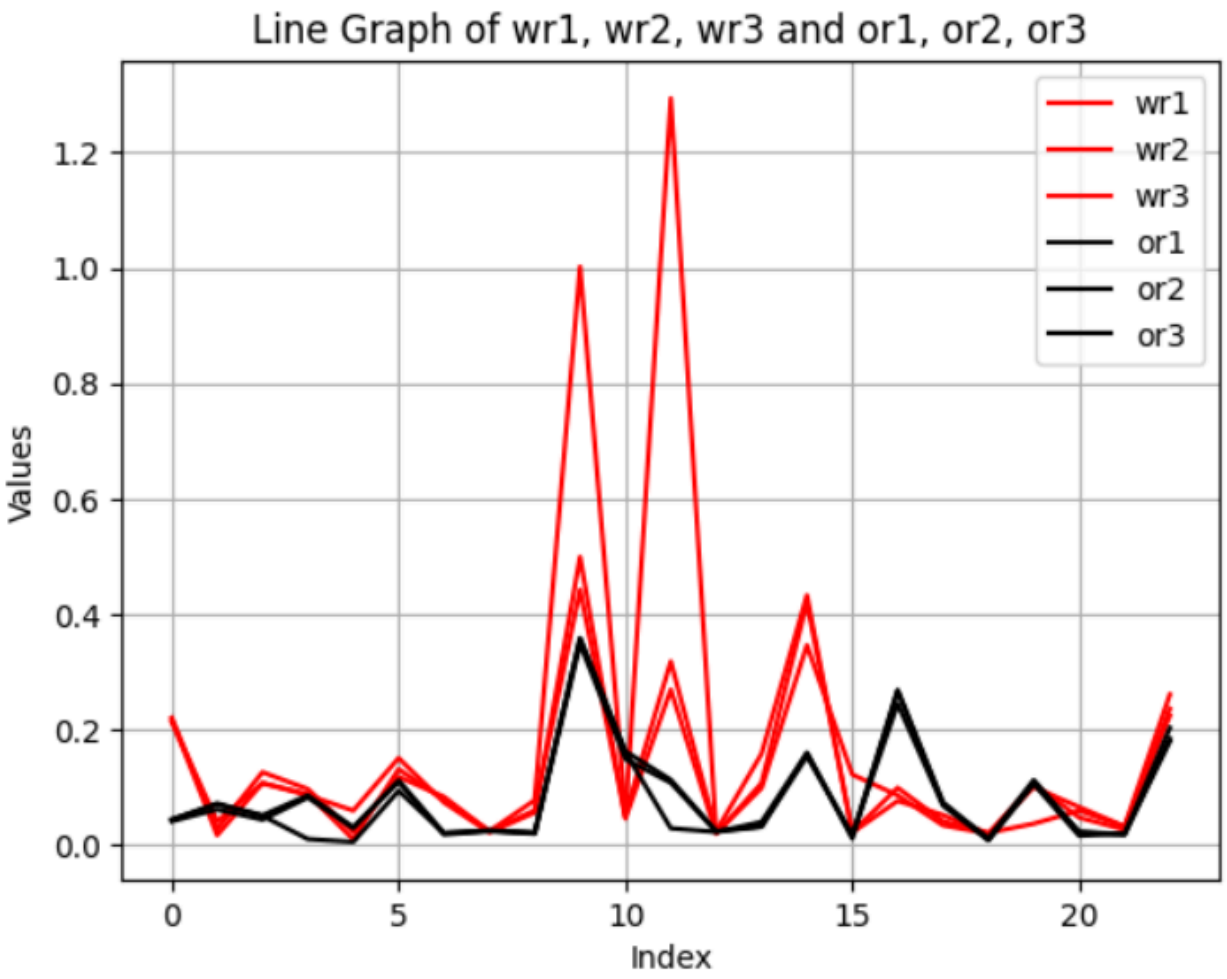


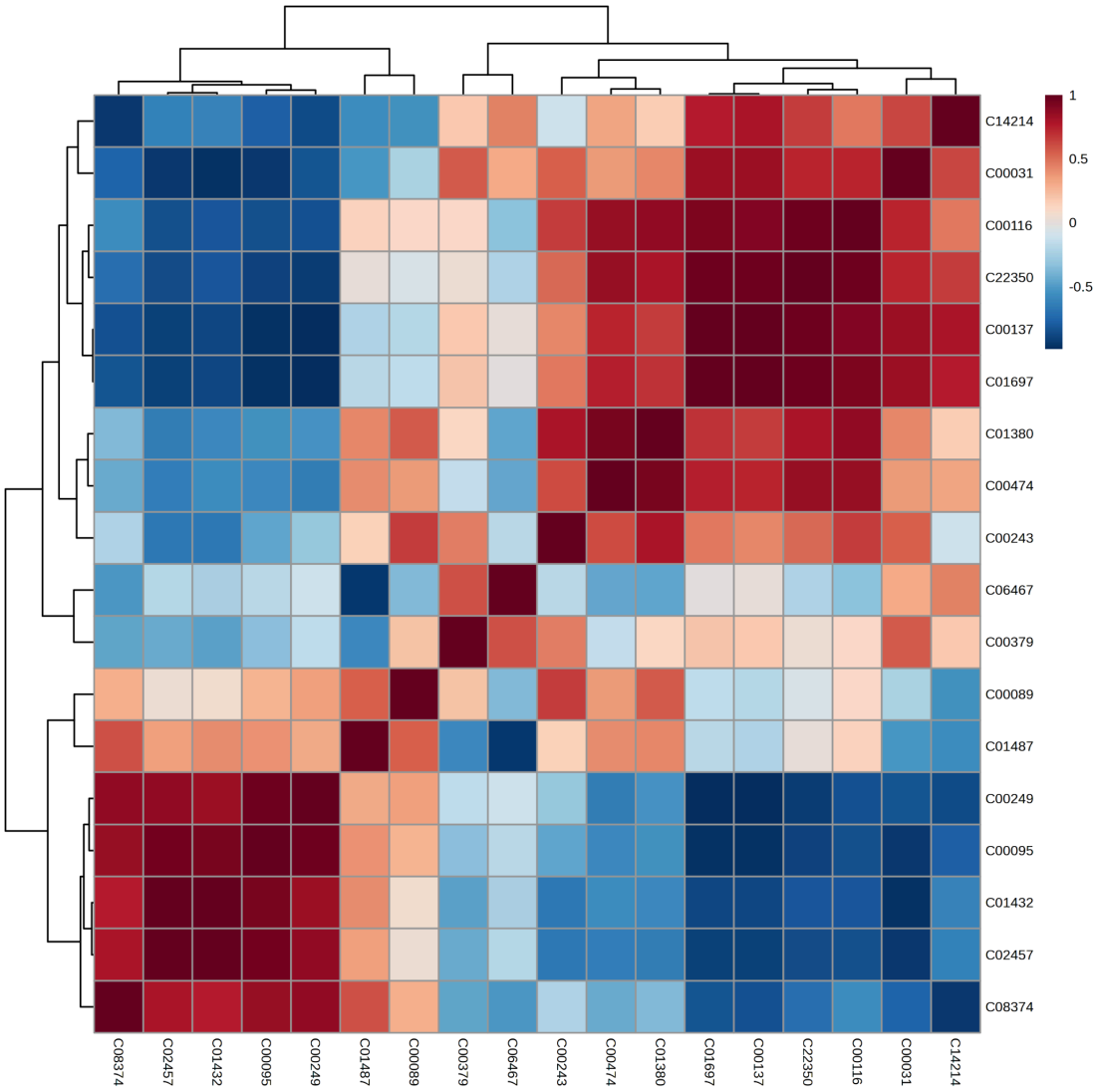
UMAP tends to preserve the local structure of the data, meaning that nearby points in the high-dimensional space are likely to be close to each other in the UMAP visualization. Therefore, clusters of points in the UMAP plot may represent clusters or groups of similar data points in the original high-dimensional space.

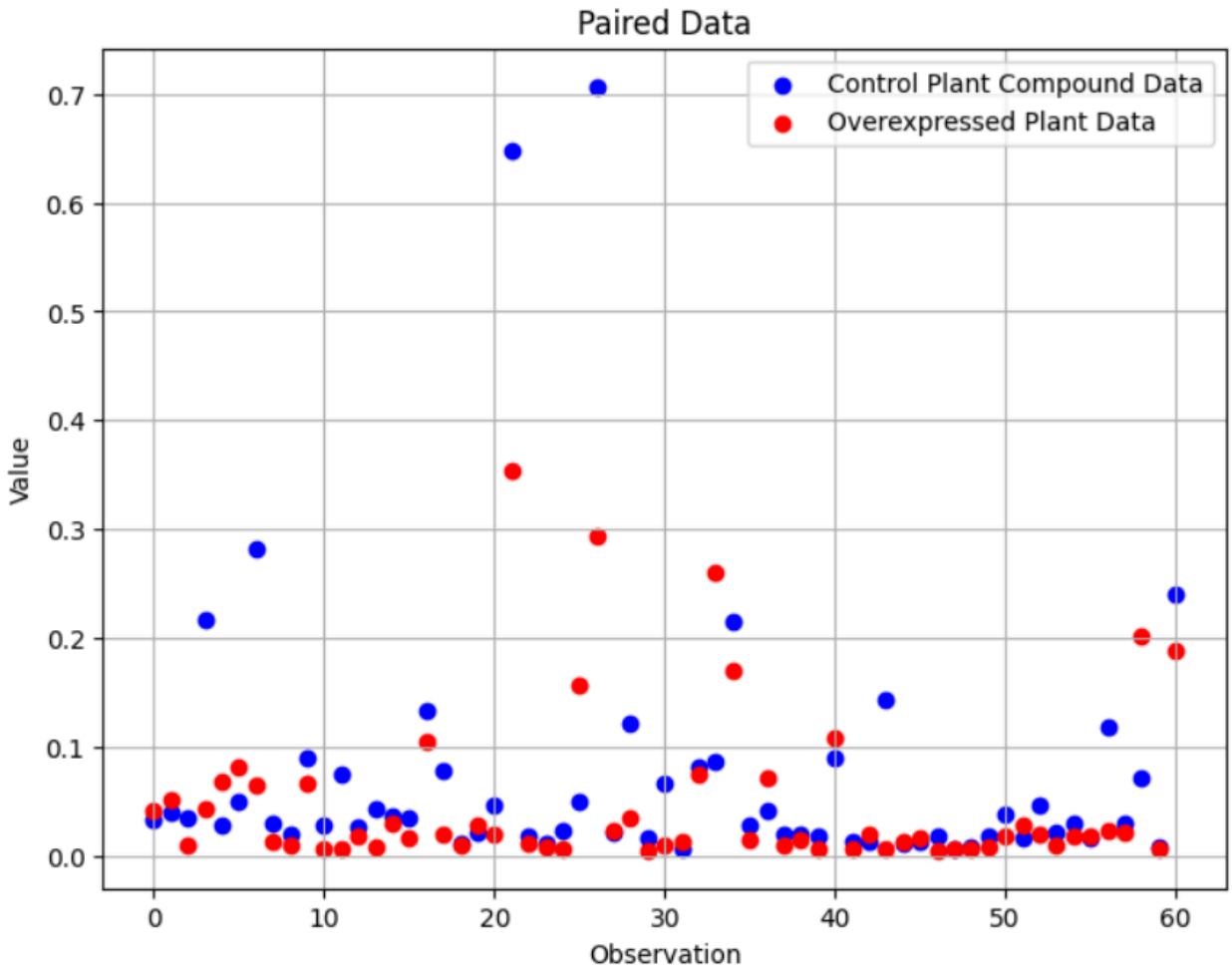
The clustering of compounds obtained through UMAP analysis of the 2D data from control and overexpressed plants holds significant implications for understanding plant biology and genetic manipulation. These clusters not only indicate similarities in chemical composition and properties but also offer insights into the underlying biological mechanisms, potentially corresponding to biochemical pathways or functional groups. Moreover, the identification of compounds clustering together provides a basis for pinpointing candidate biomarkers that can distinguish between control and overexpressed plants, guiding further investigation into their roles in plant physiology or response to overexpression. By focusing on compounds within specific clusters, researchers can conduct targeted analyses and experimental validations, deepening our understanding of their biological significance and implications for plant genetic manipulation.

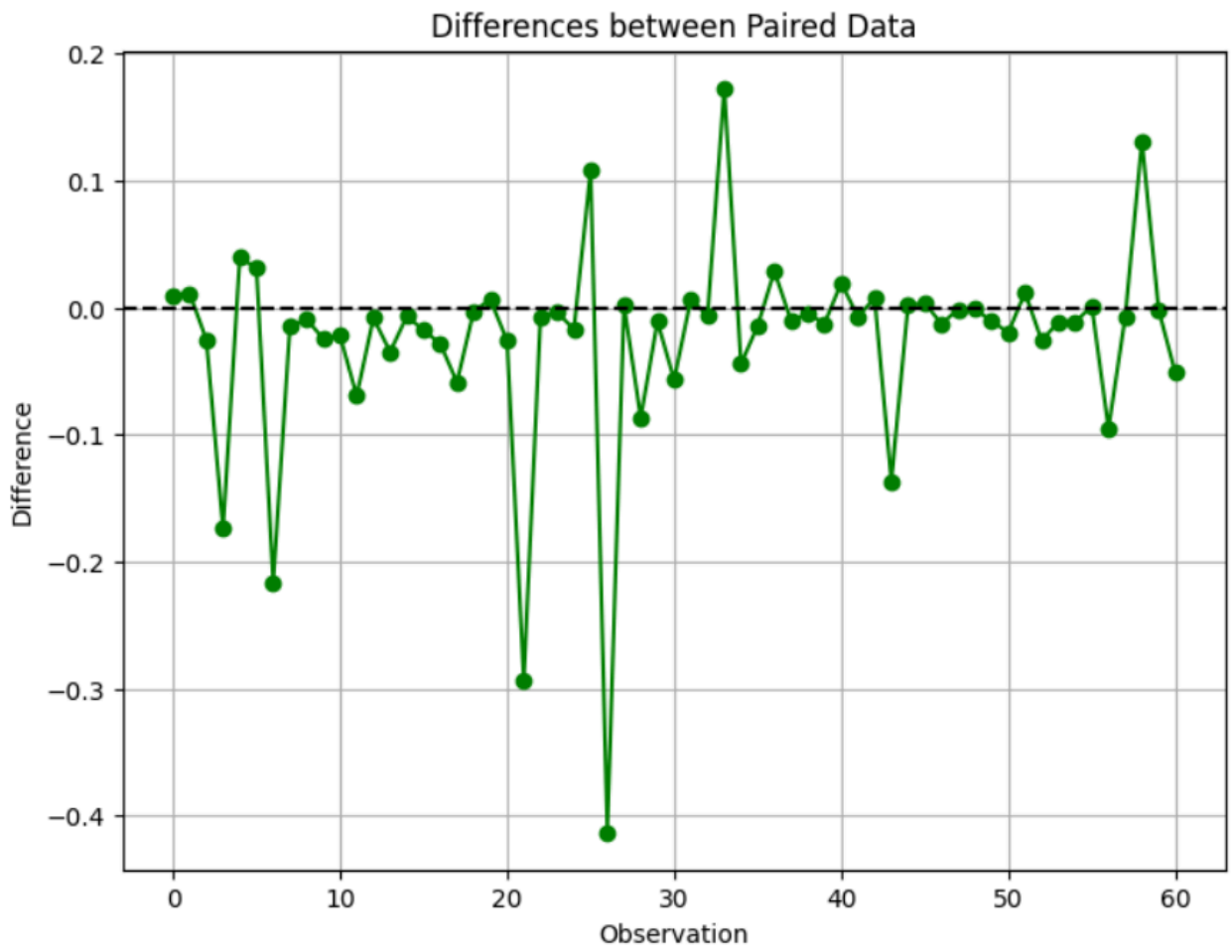
Moreover, the identification of compounds clustering together offers a promising avenue for identifying candidate biomarkers that can effectively discriminate between control and overexpressed plants. These biomarkers may serve as indicators of physiological changes induced by genetic manipulation, facilitating the development of novel strategies for crop improvement and biotechnology applications. Furthermore, by focusing on compounds within specific clusters, researchers can conduct targeted analyses and experimental validations to elucidate their biological roles and functional significance.

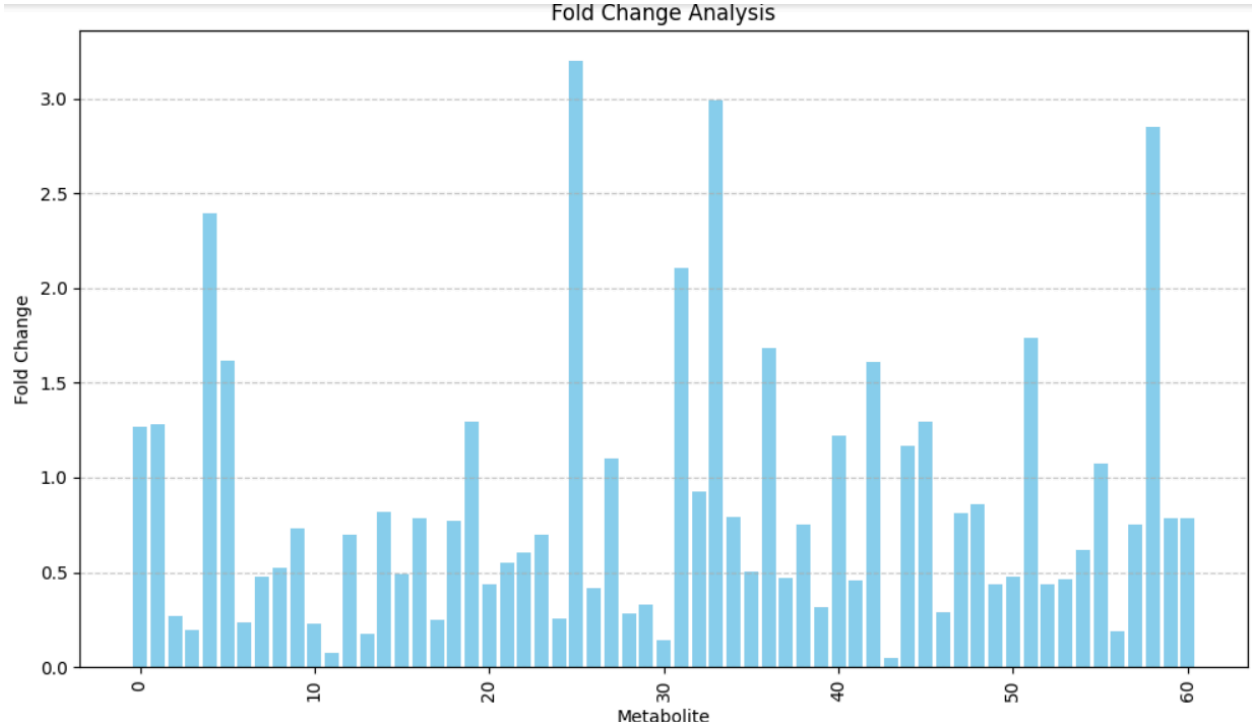


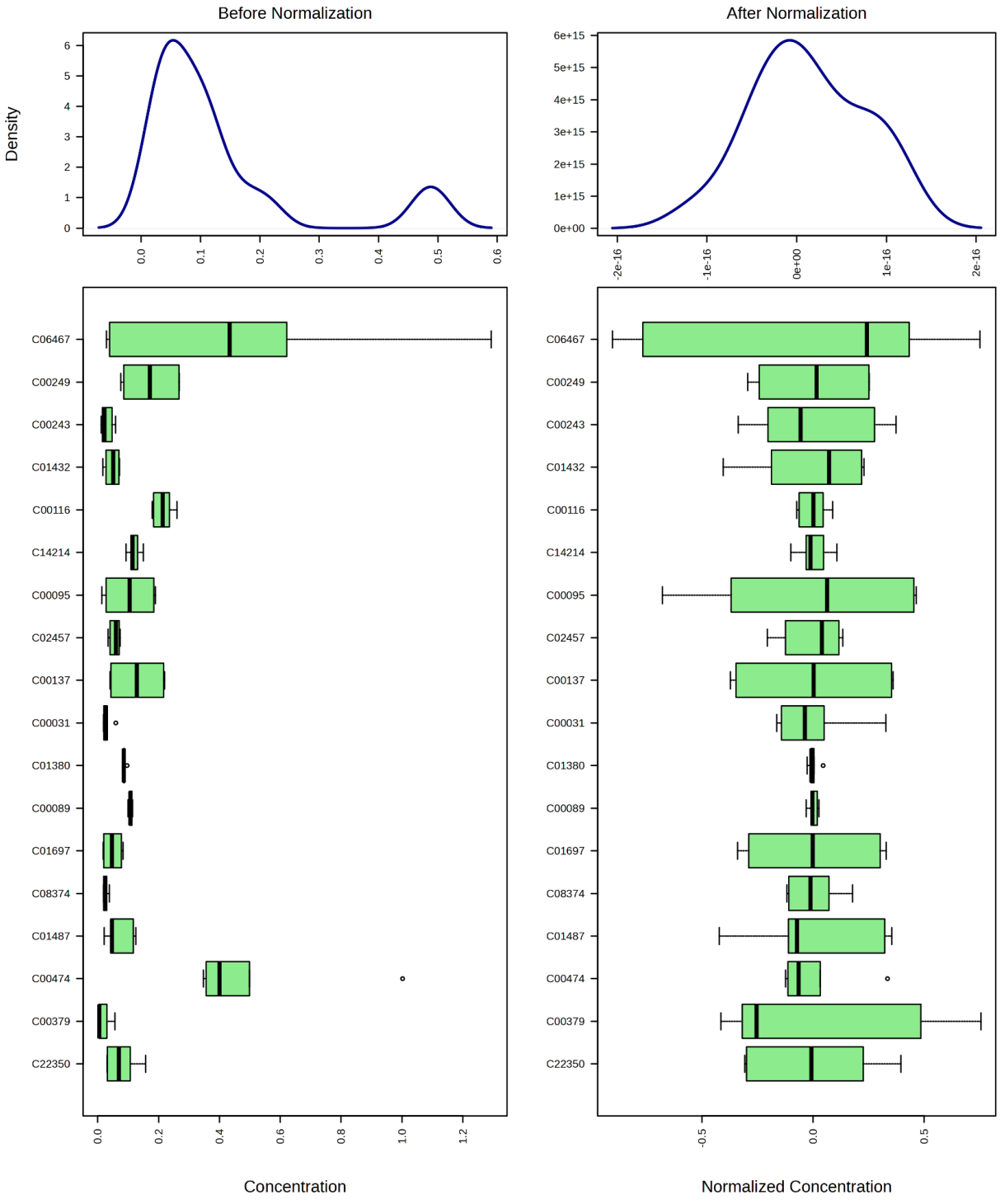

Line Graph of wr1, wr2, wr3 and or1, or2, or3
wr1
wr2
wr3
or1
or2
or3
Values
Index
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
5
10
15
20

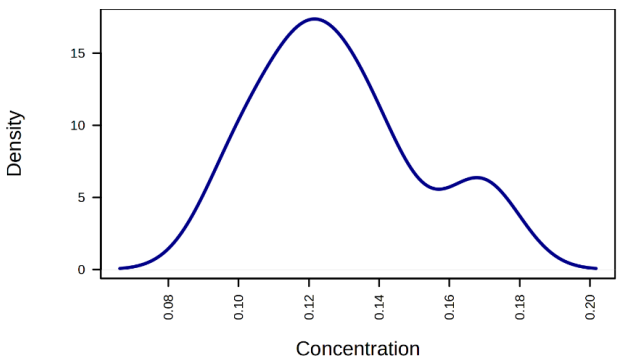

C14214
C00031
C00116
C22350
C00137
C01697
C01380
C00474
C00243
C06467
C00379
C00089
C01487
C00249
C00095
C01432
C02457
C08374
1
0.5
0
-0.5

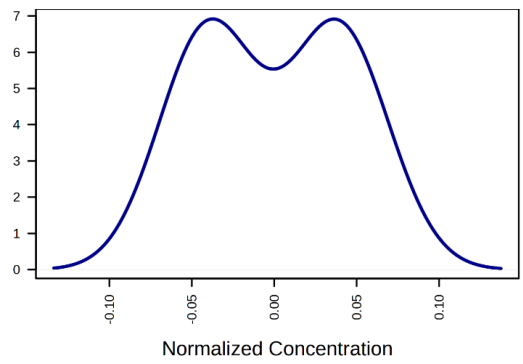

Paired Data
Control Plant Compound Data
Overexpressed Plant Data
Value
Observation
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
10
20
30
40
50
60

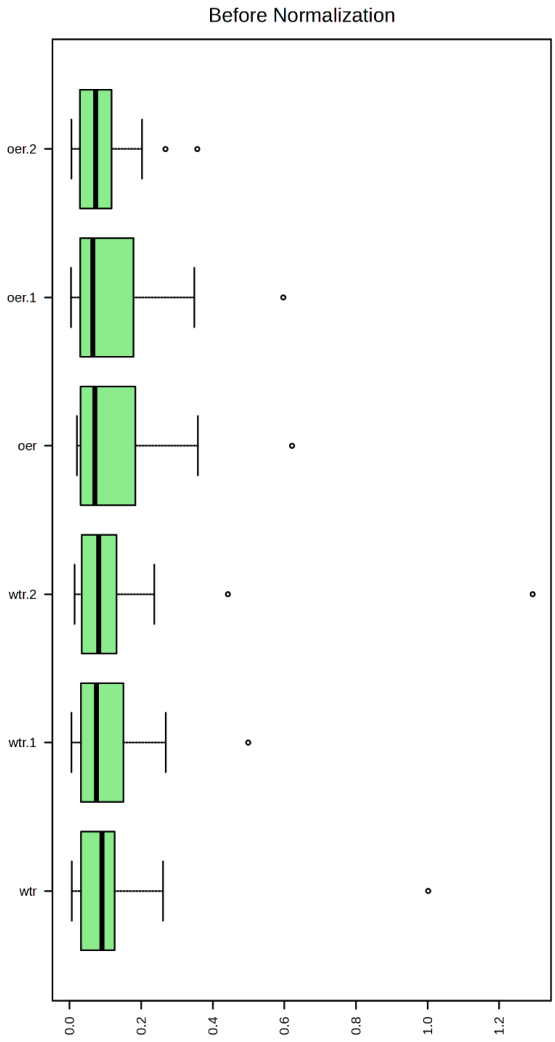

Differences between Paired Data
Difference
Observation
0.2
0.1
0.0
−0.1
−0.2
−0.3
−0.4
0
10
20
30
40
50
60

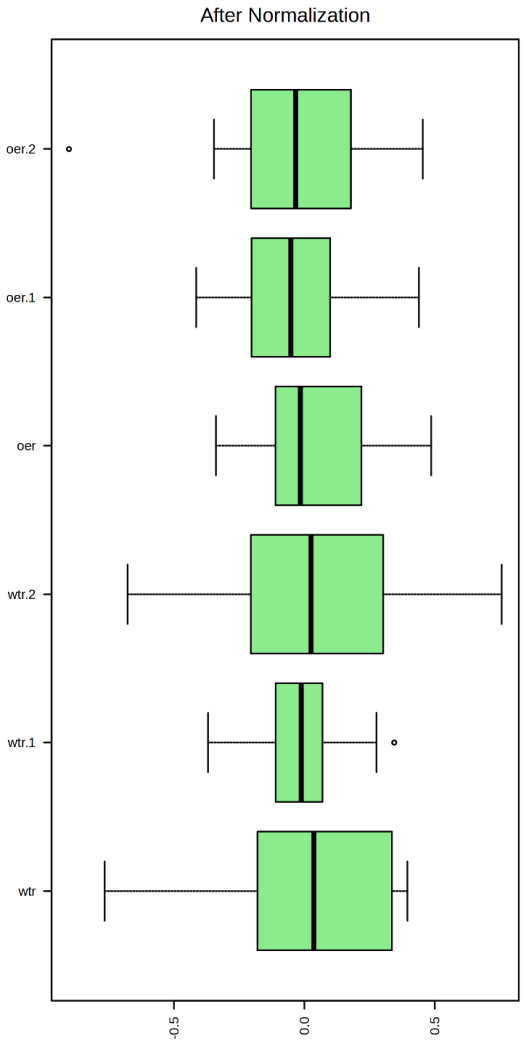

Fold Change Analysis
Fold Change
Metabolite
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
10
20
30
40
50
60


Before Normalization
After Normalization
Density
0
1
2
3
4
5
6
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0e+00
1e+15
2e+15
3e+15
4e+15
5e+15
6e+15
-2e-16
-1e-16
0e+00
1e-16
2e-16
C06467
C00249
C00243
C01432
C00116
C14214
C00095
C02457
C00137
C00031
C01380
C00089
C01697
C08374
C01487
C00474
C00379
C22350
0.0
0.2
0.4
0.6
0.8
1.0
1.2
-0.5
0.0
0.5
Concentration
Normalized Concentration


Density
15
10
5
0
0.08
0.10
0.12
0.14
0.16
0.18
0.20
Concentration


7
6
5
4
3
2
1
0
-0.10
-0.05
0.00
0.05
0.10
Normalized Concentration


Before Normalization
oer.2
oer.1
oer
wtr.2
wtr.1
wtr
0.0
0.2
0.4
0.6
0.8
1.0
1.2


After Normalization
oer.2
oer.1
oer
wtr.2
wtr.1
wtr
-0.5
0.0
0.5