Figures:

Figure 1

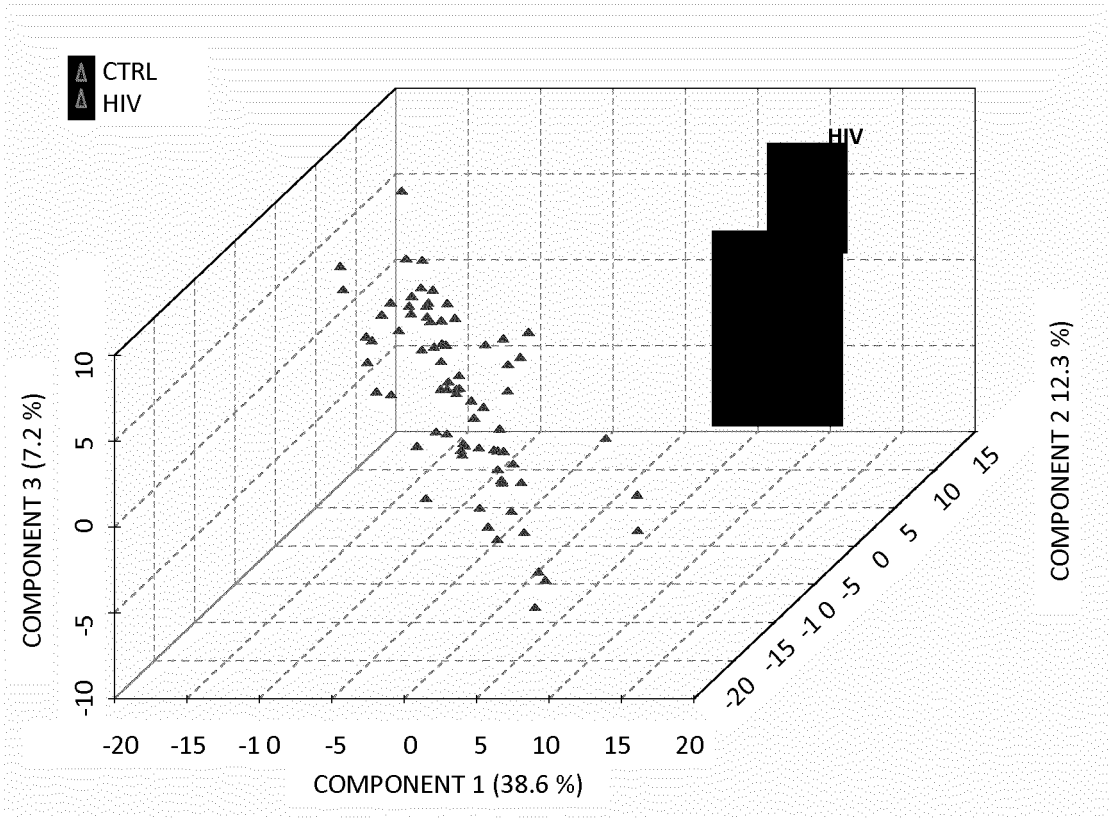


Figure 2A

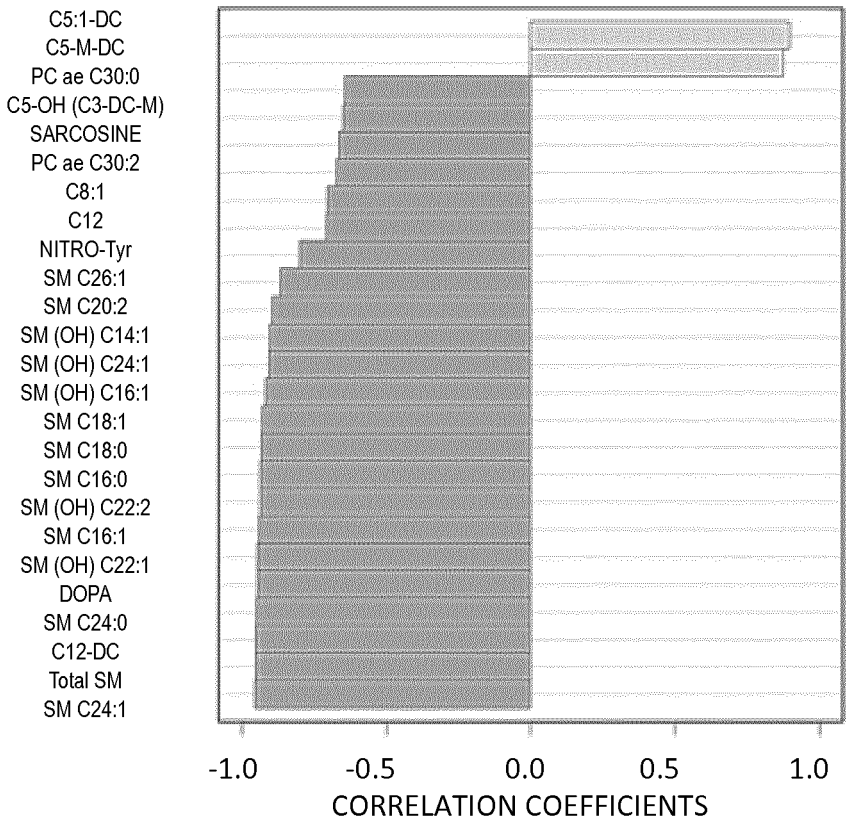

C5:1-DC
C5-M-DC
PC ae C30:0
C5-OH (C3-DC-M)
SARCOSINE
PC ae C30:2
C8:1
C12
NITRO-Tyr
SM C26:1
SM C20:2
SM (OH) C14:1
SM (OH) C24:1
SM (OH) C16:1
SM C18:1
SM C18:0
SM C16:0
SM (OH) C22:2
SM C16:1
SM (OH) C22:1
DOPA
SM C24:0
C12-DC
Total SM
SM C24:1
-1.0
-0.5
0.0
0.5
1.0
CORRELATION COEFFICIENTS

Figure 2B

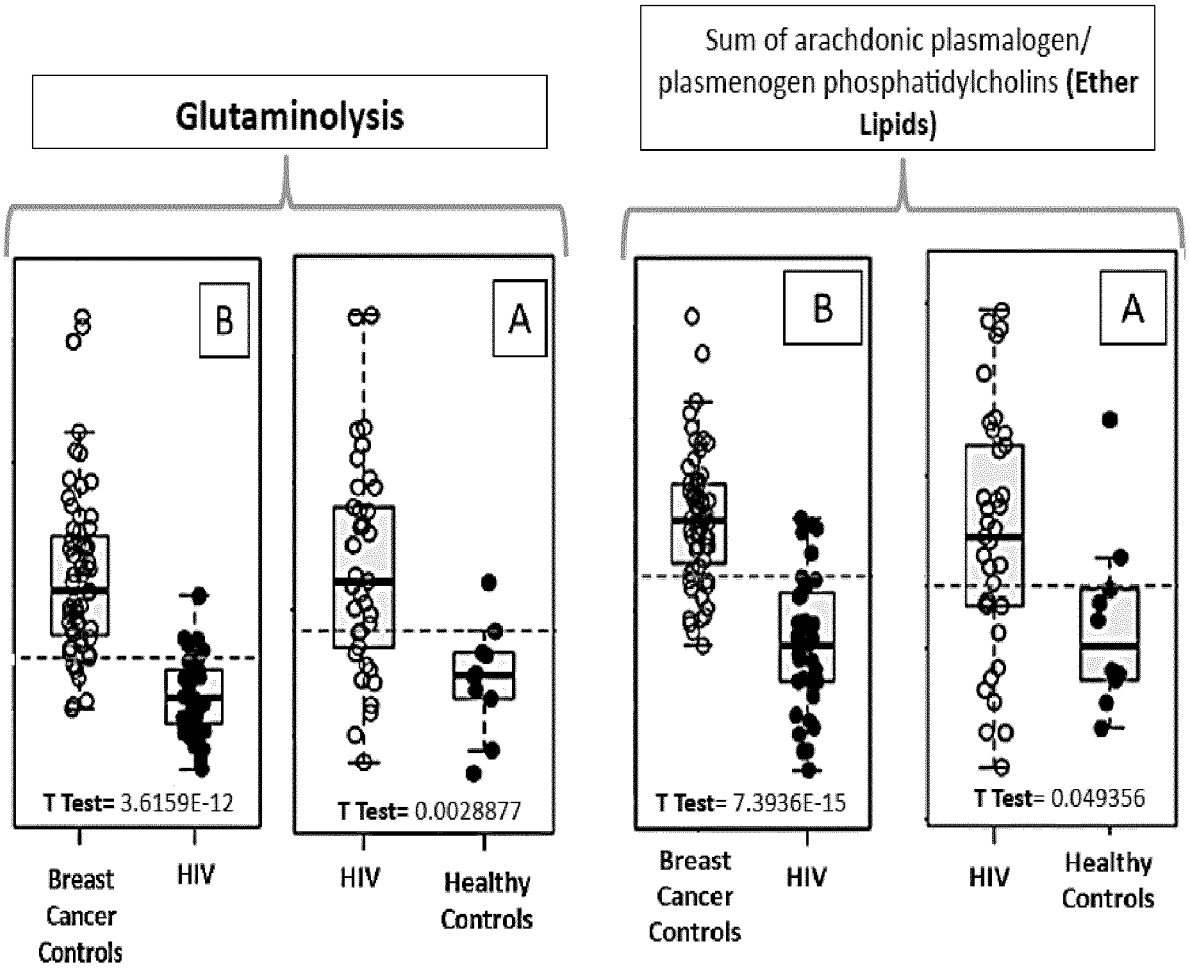

Glutaminolysis
Sum of arachdonic plasmalogen/ plasmenogen phosphatidylcholins (Ether Lipids)
B
A
B
A
T Test= 3.6159E-12
T Test= 0.0028877
T Test= 7.3936E-15
T Test= 0.049356
Breast Cancer Controls
HIV
HIV
Healthy Controls
Breast Cancer Controls
HIV
HIV
Healthy Controls

Figure 3.1

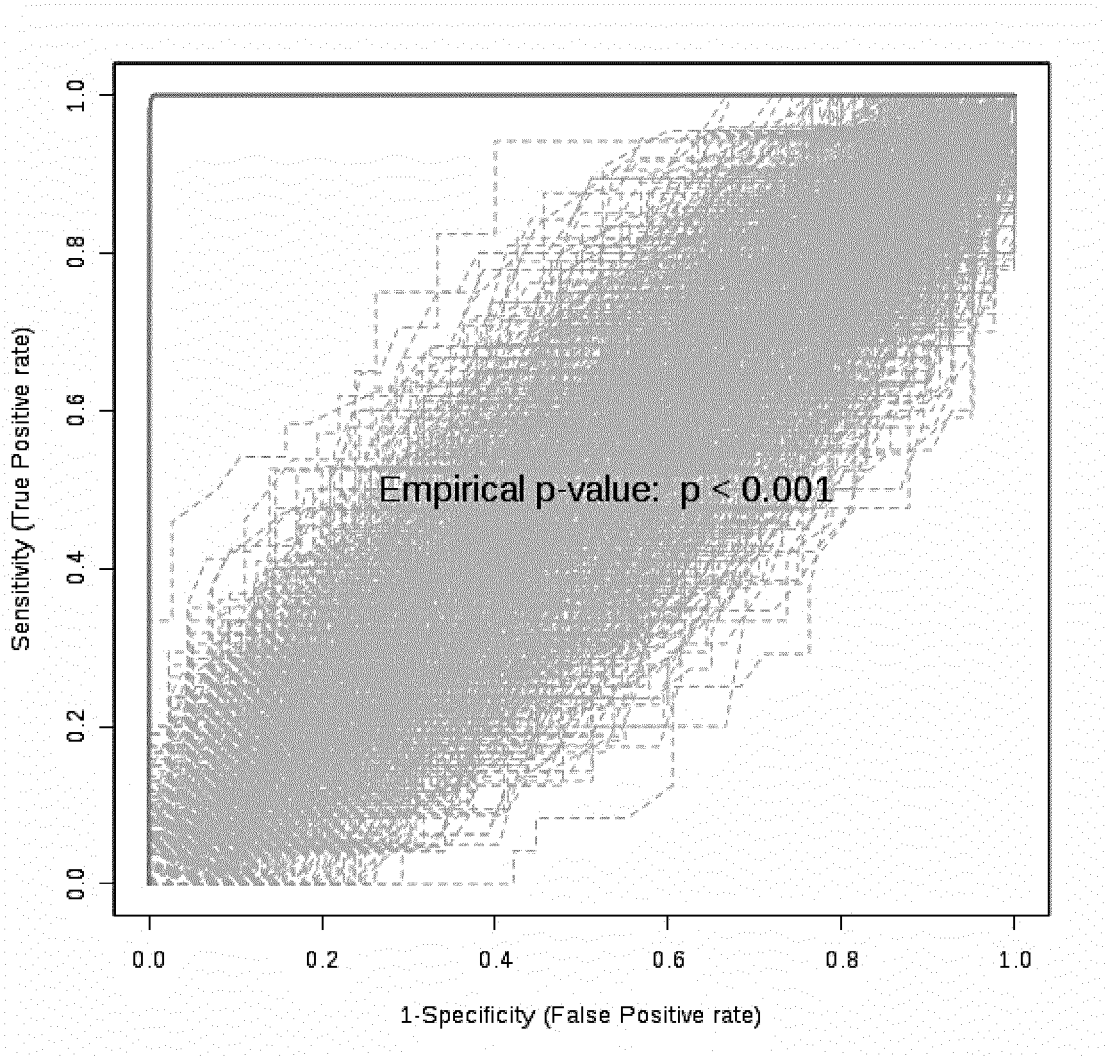

Empirical p-value: p < 0.001
Sensitivity (True Positive rate)
1-Specificity (False Positive rate)
0.0
0.2
0.4
0.6
0.8
1.0

Figure 3.2

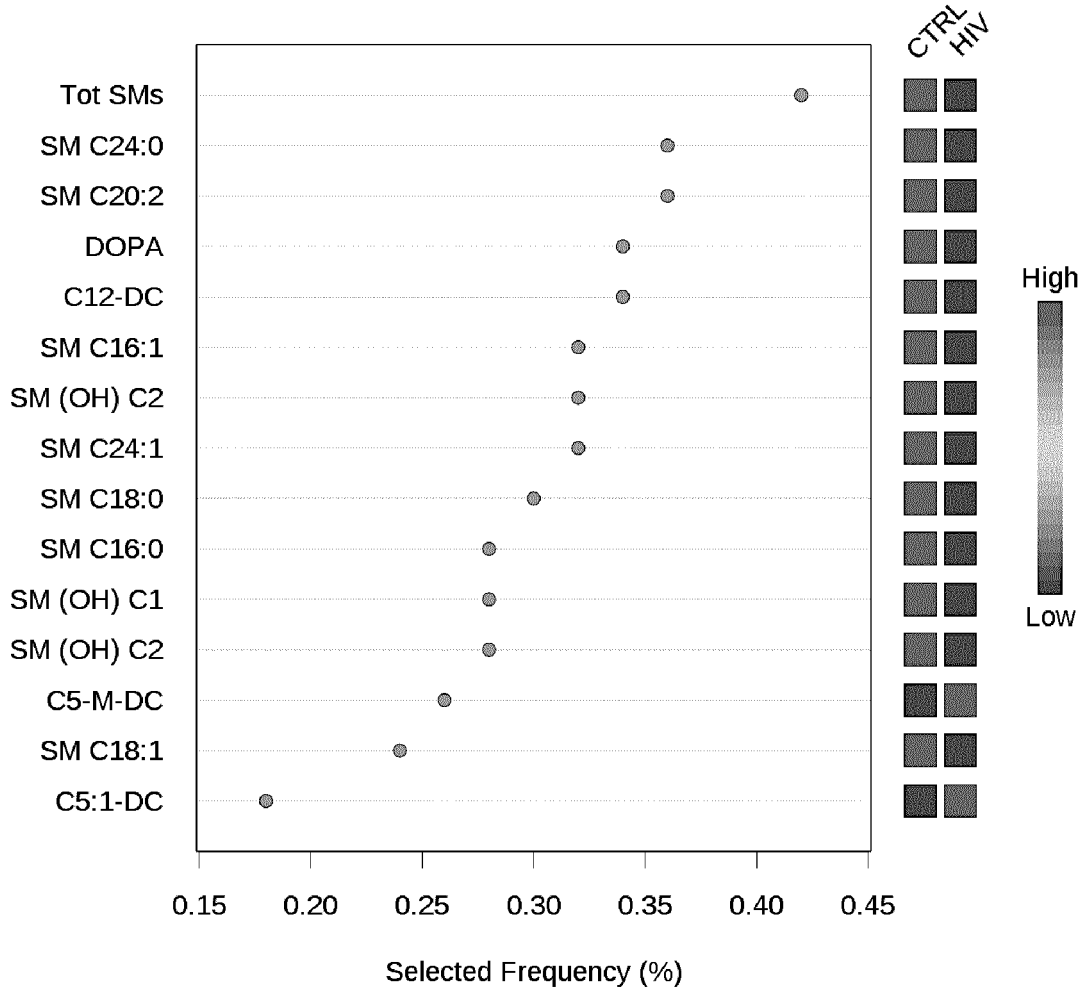

CTRL
HIV
Tot SMs
SM C24:0
SM C20:2
DOPA
C12-DC
SM C16:1
SM (OH) C2
SM C24:1
SM C18:0
SM C16:0
SM (OH) C1
SM (OH) C2
C5-M-DC
SM C18:1
C5:1-DC
High
Low
0.15
0.20
0.25
0.30
0.35
0.40
0.45
Selected Frequency (%)

Figure 4A1

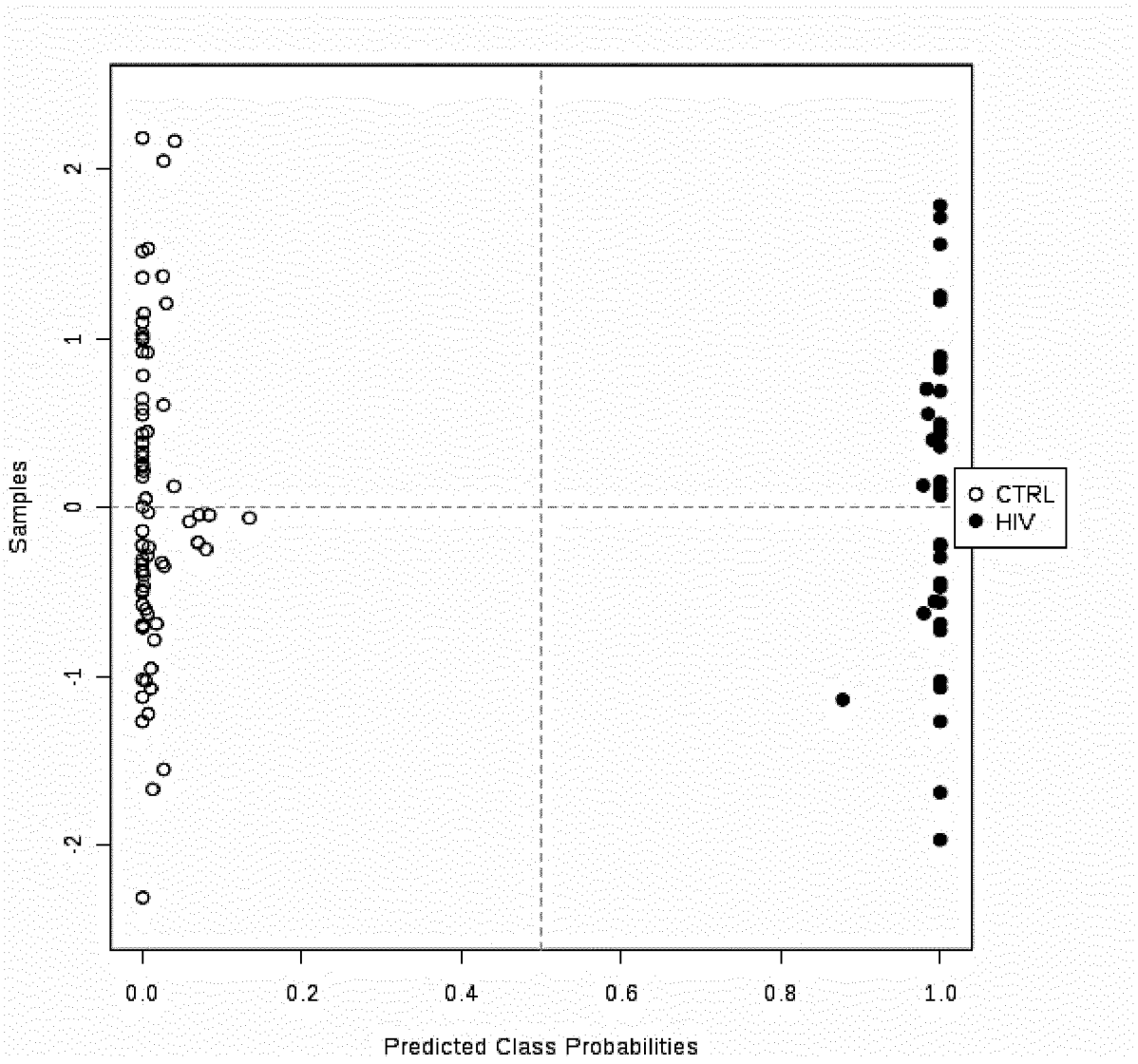

Samples
2
1
0
-1
-2
0.0
0.2
0.4
0.6
0.8
1.0
Predicted Class Probabilities
CTRL
HIV

Figure 4A.2

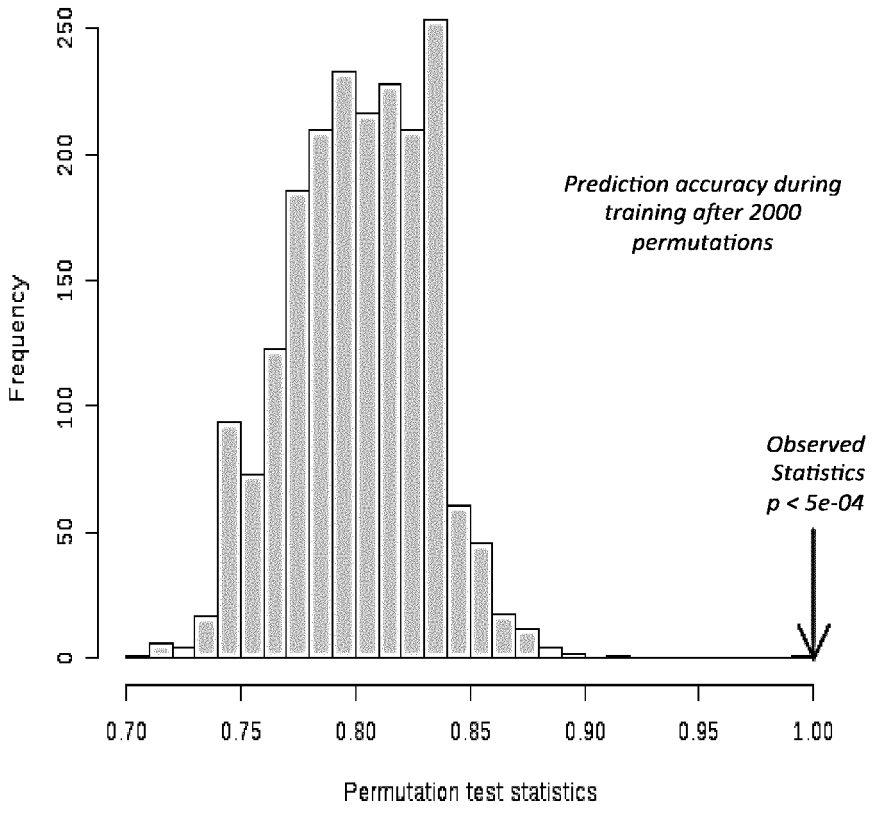

Frequency
0
50
100
150
200
250
Prediction accuracy during training after 2000 permutations
Observed Statistics
p < 5e-04
0.70
0.75
0.80
0.85
0.90
0.95
1.00
Permutation test statistics

Figure 4B

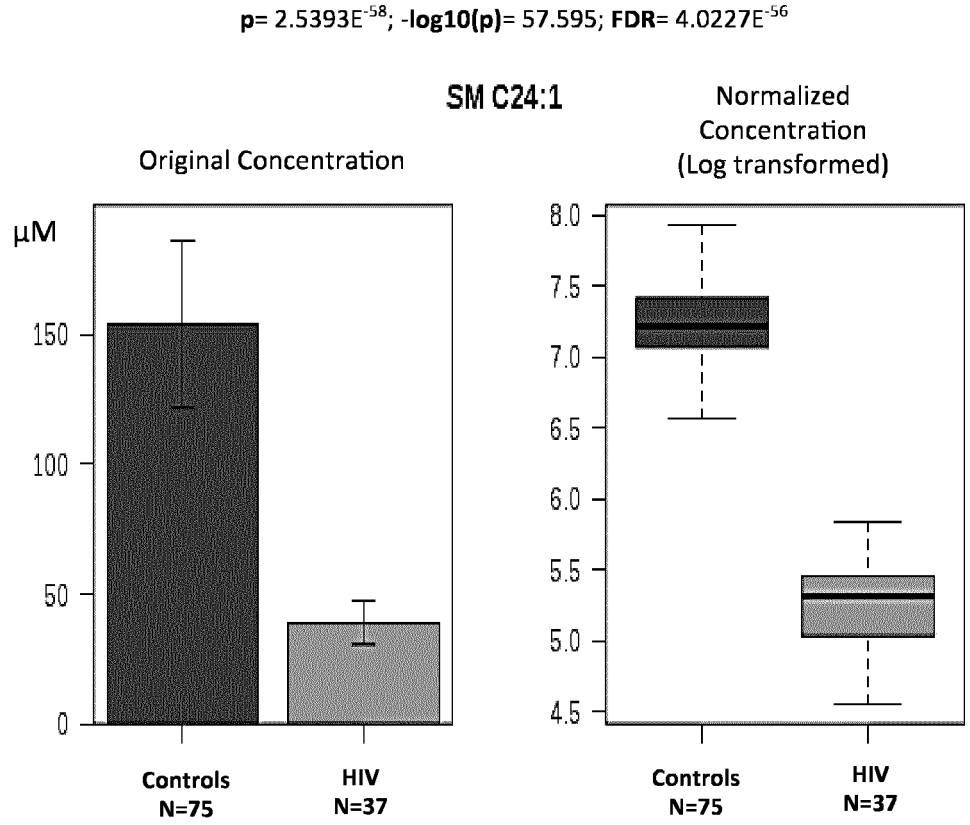

p= 2.5393E-58; -log10(p)= 57.595; FDR= 4.0227E-56
SM C24:1
Original Concentration
µM
150
100
50
0
Controls N=75
HIV N=37
Normalized Concentration (Log transformed)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
Controls N=75
HIV N=37

Figure 4C

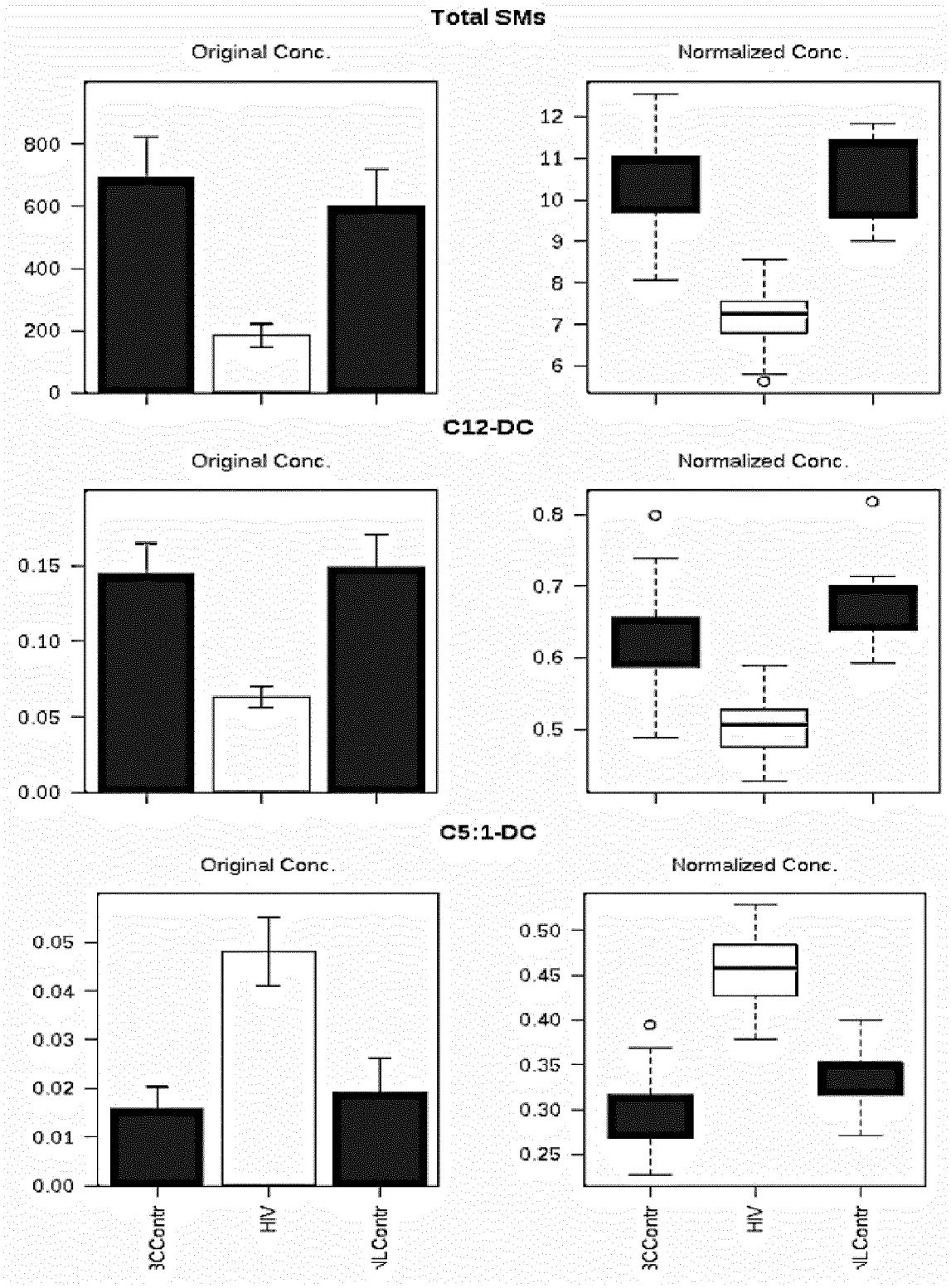

Total SMs
Original Conc.
Normalized Conc.
800
600
400
200
0
12
11
10
9
8
7
6
C12-DC
Original Conc.
Normalized Conc.
0.15
0.10
0.05
0.00
0.8
0.7
0.6
0.5
C5:1-DC
Original Conc.
Normalized Conc.
0.05
0.04
0.03
0.02
0.01
0.00
0.50
0.45
0.40
0.35
0.30
0.25
HIV

Figure 5A

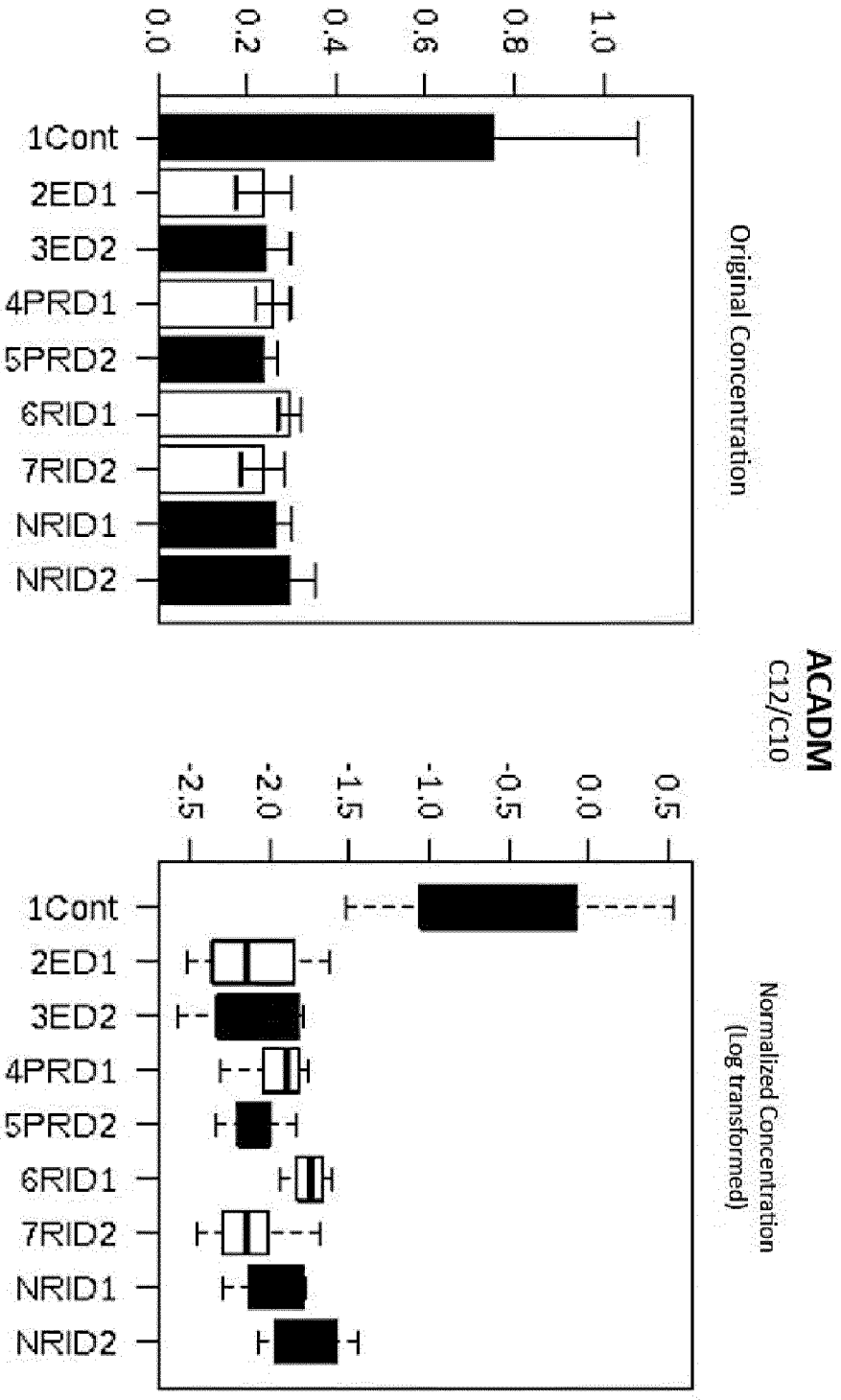

ACADM
C12/C10
0.0
0.2
0.4
0.6
0.8
1.0
1Cont
2ED1
3ED2
4PRD1
5PRD2
6RID1
7RID2
NRID1
NRID2
Original Concentration
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1Cont
2ED1
3ED2
4PRD1
5PRD2
6RID1
7RID2
NRID1
NRID2
Normalized Concentration
(Log transformed)

Figure 5B

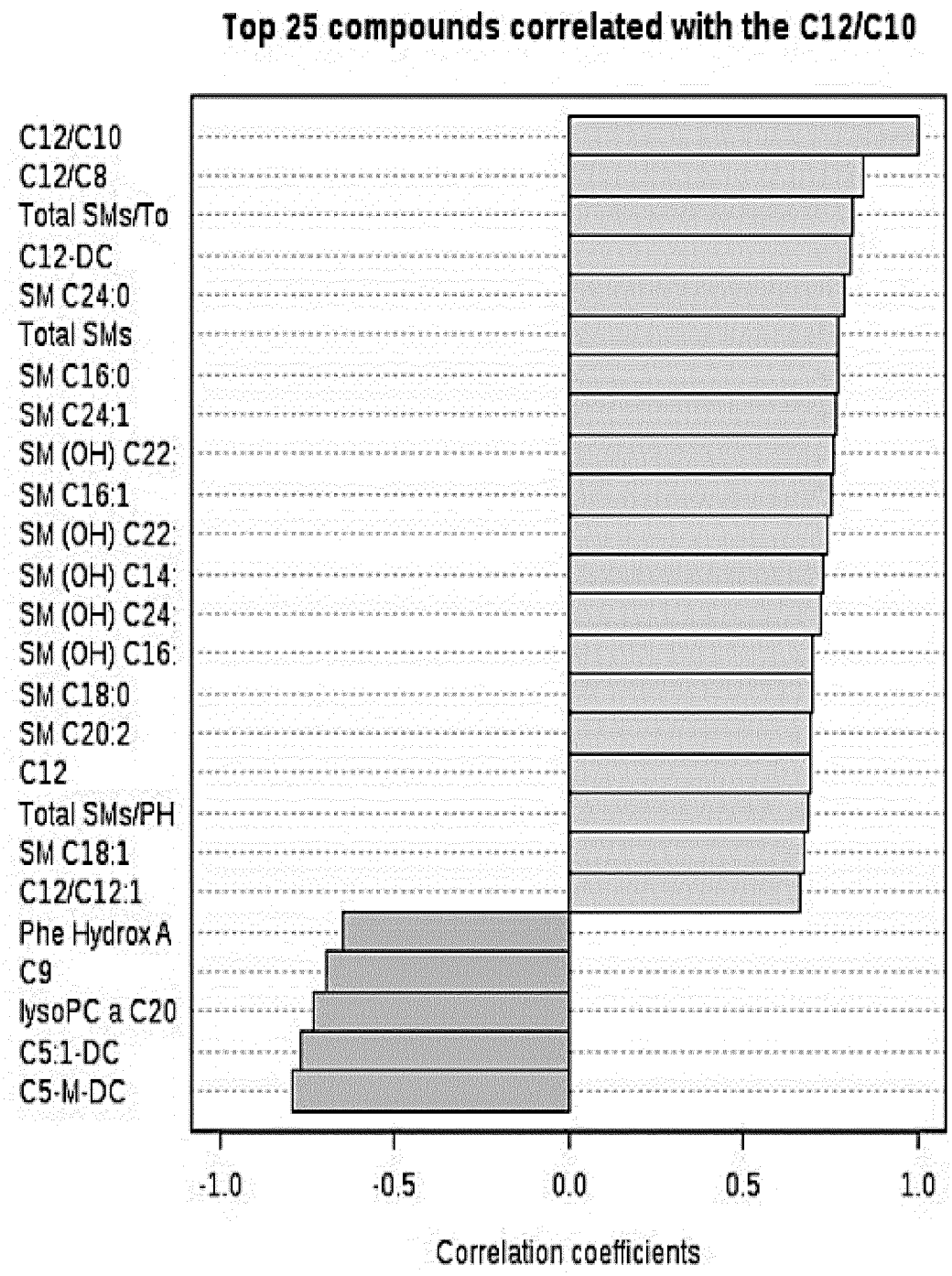

Top 25 compounds correlated with the C12/C10
C12/C10
C12/C8
Total SMs/To
C12-DC
SM C24:0
Total SMs
SM C16:0
SM C24:1
SM (OH) C22:
SM C16:1
SM (OH) C22:
SM (OH) C14:
SM (OH) C24:
SM (OH) C16:
SM C18:0
SM C20:2
C12
Total SMs/PH
SM C18:1
C12/C12:1
Phe Hydrox A
C9
lysoPC a C20
C5:1-DC
C5-M-DC
-1.0
-0.5
0.0
0.5
1.0
Correlation coefficients

Figure 6A

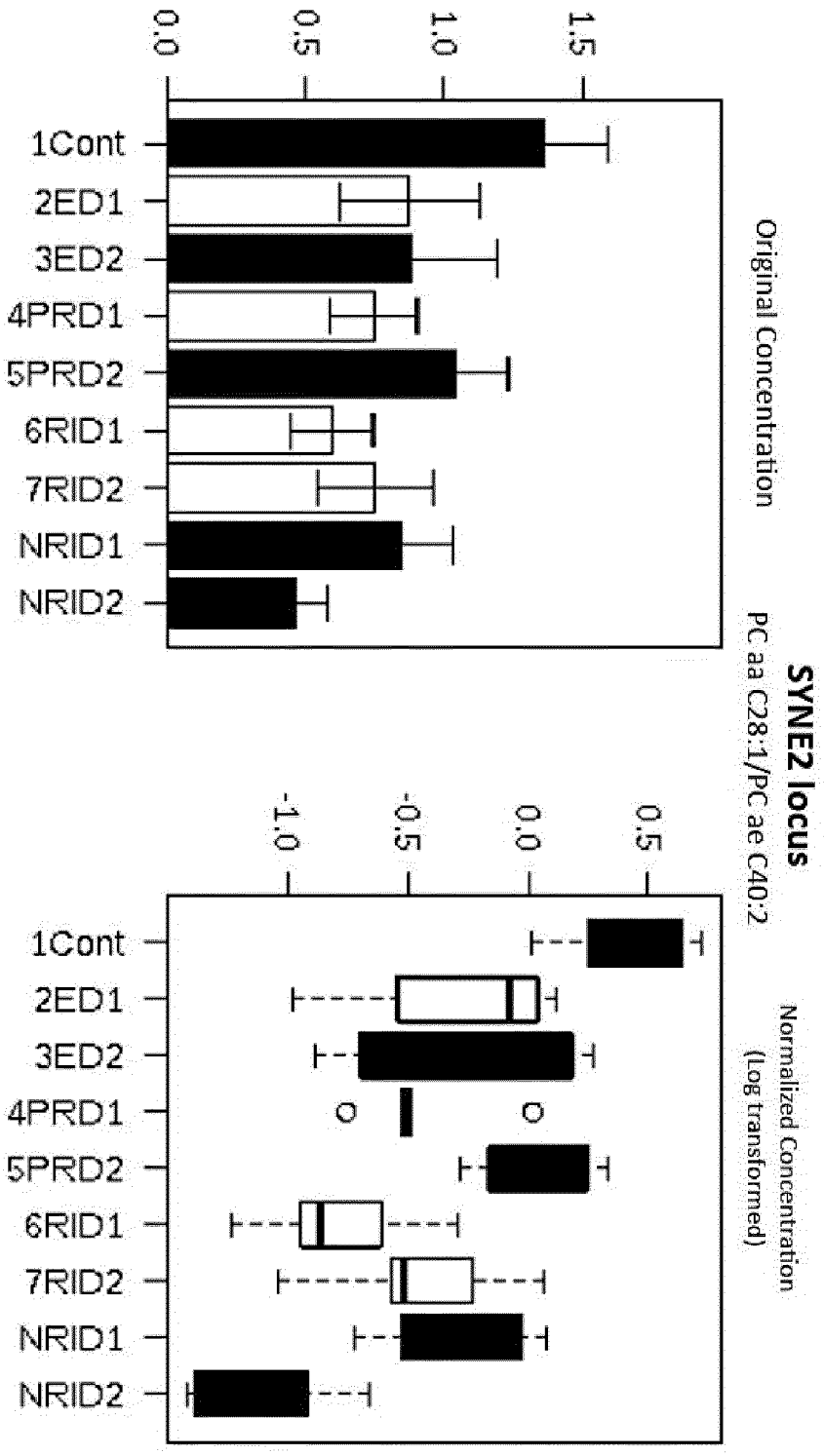

SYNE2 locus
PC aa C28:1/PC ae C40:2
Original Concentration
0.0
0.5
1.0
1.5
1Cont
2ED1
3ED2
4PRD1
5PRD2
6RID1
7RID2
NRID1
NRID2
Normalized Concentration
(Log transformed)
-1.0
-0.5
0.0
0.5
1Cont
2ED1
3ED2
4PRD1
5PRD2
6RID1
7RID2
NRID1
NRID2

Figure 6B

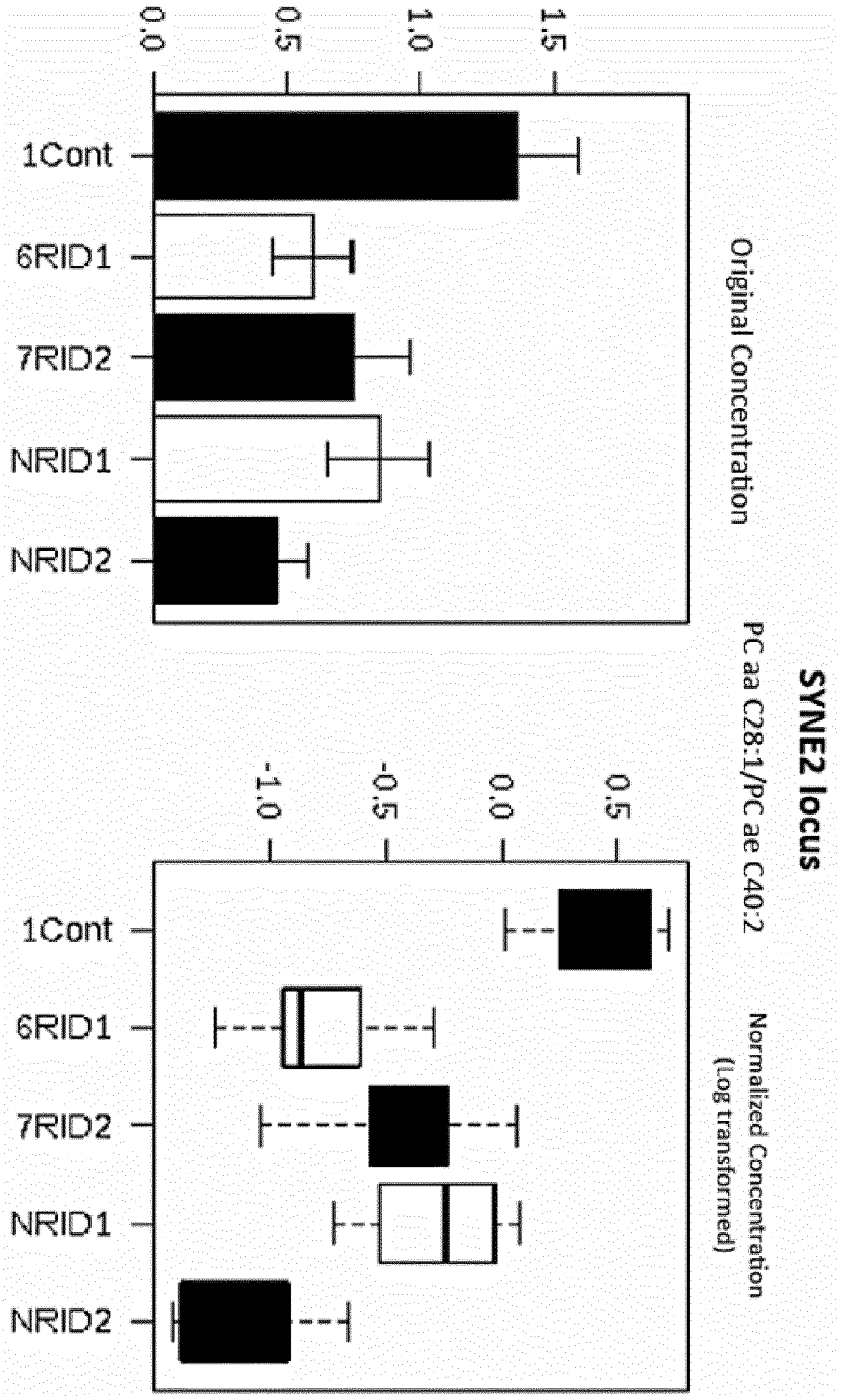

SYNE2 locus
PC aa C28:1/PC ae C40:2
Original Concentration
0.0
0.5
1.0
1.5
1Cont
6RID1
7RID2
NRID1
NRID2
Normalized Concentration
(Log transformed)
-1.0
-0.5
0.0
0.5
1Cont
6RID1
7RID2
NRID1
NRID2

Figure 6C

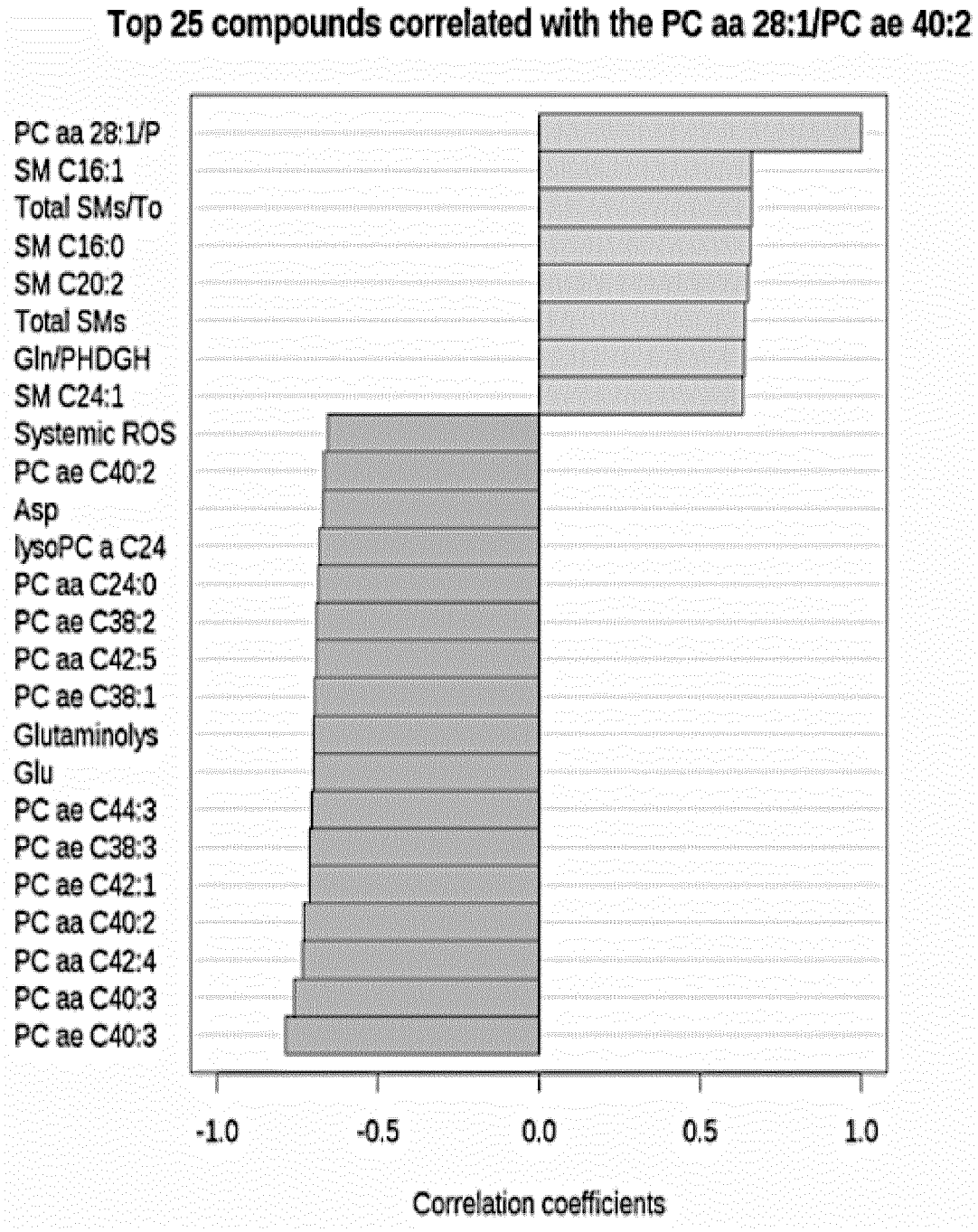

Top 25 compounds correlated with the PC aa 28:1/PC ae 40:2
PC aa 28:1/P
SM C16:1
Total SMs/To
SM C16:0
SM C20:2
Total SMs
Gln/PHDGH
SM C24:1
Systemic ROS
PC ae C40:2
Asp
lysoPC a C24
PC aa C24:0
PC ae C38:2
PC aa C42:5
PC ae C38:1
Glutaminolys
Glu
PC ae C44:3
PC ae C38:3
PC ae C42:1
PC aa C40:2
PC aa C42:4
PC aa C40:3
PC ae C40:3
-1.0
-0.5
0.0
0.5
1.0
Correlation coefficients

Figure 7A

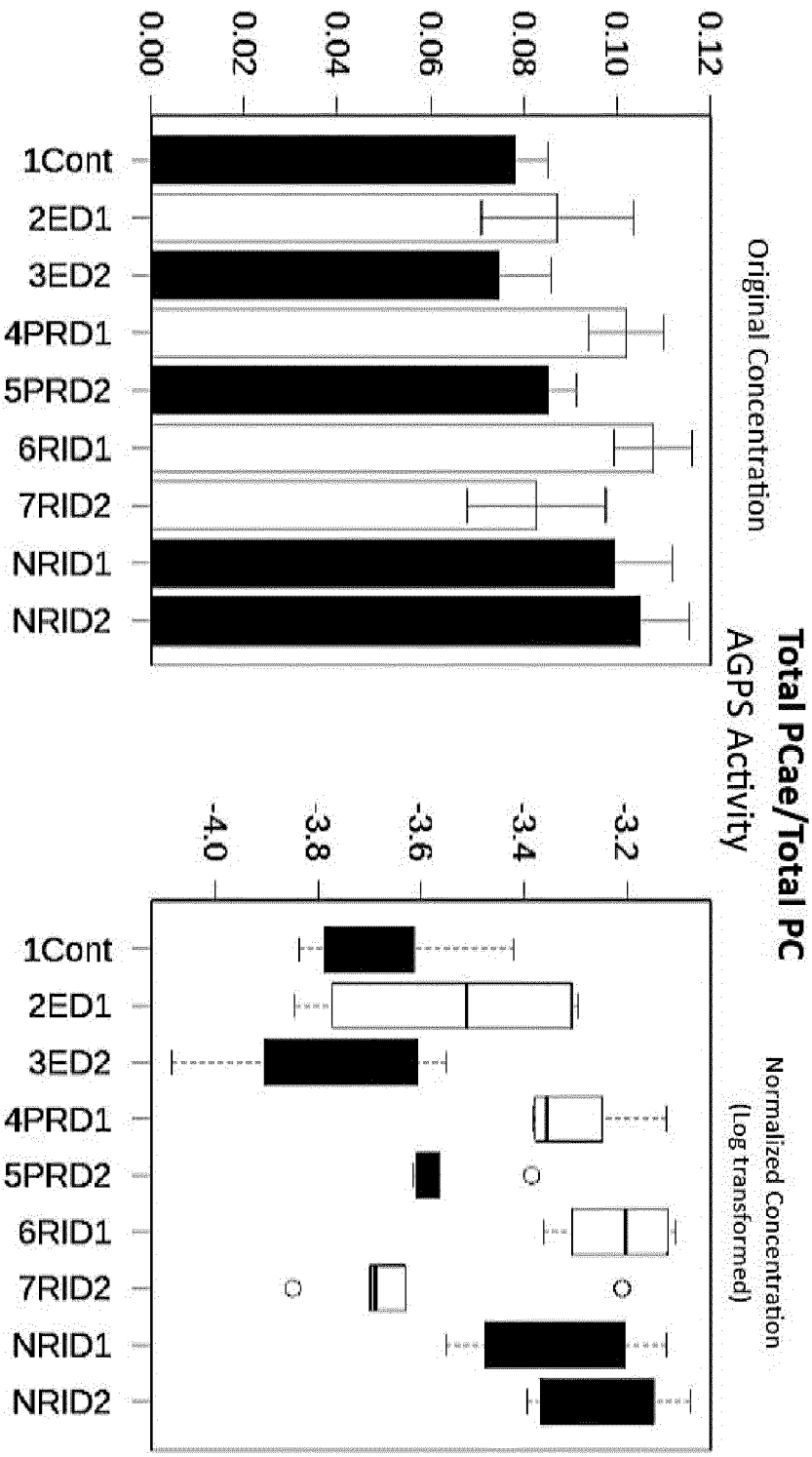

Total PCae/Total PC
AGPS Activity
Original Concentration
0.00
0.02
0.04
0.06
0.08
0.10
0.12
1Cont
2ED1
3ED2
4PRD1
5PRD2
6RID1
7RID2
NRID1
NRID2
Normalized Concentration
(Log transformed)
-4.0
-3.8
-3.6
-3.4
-3.2

Figure 7B

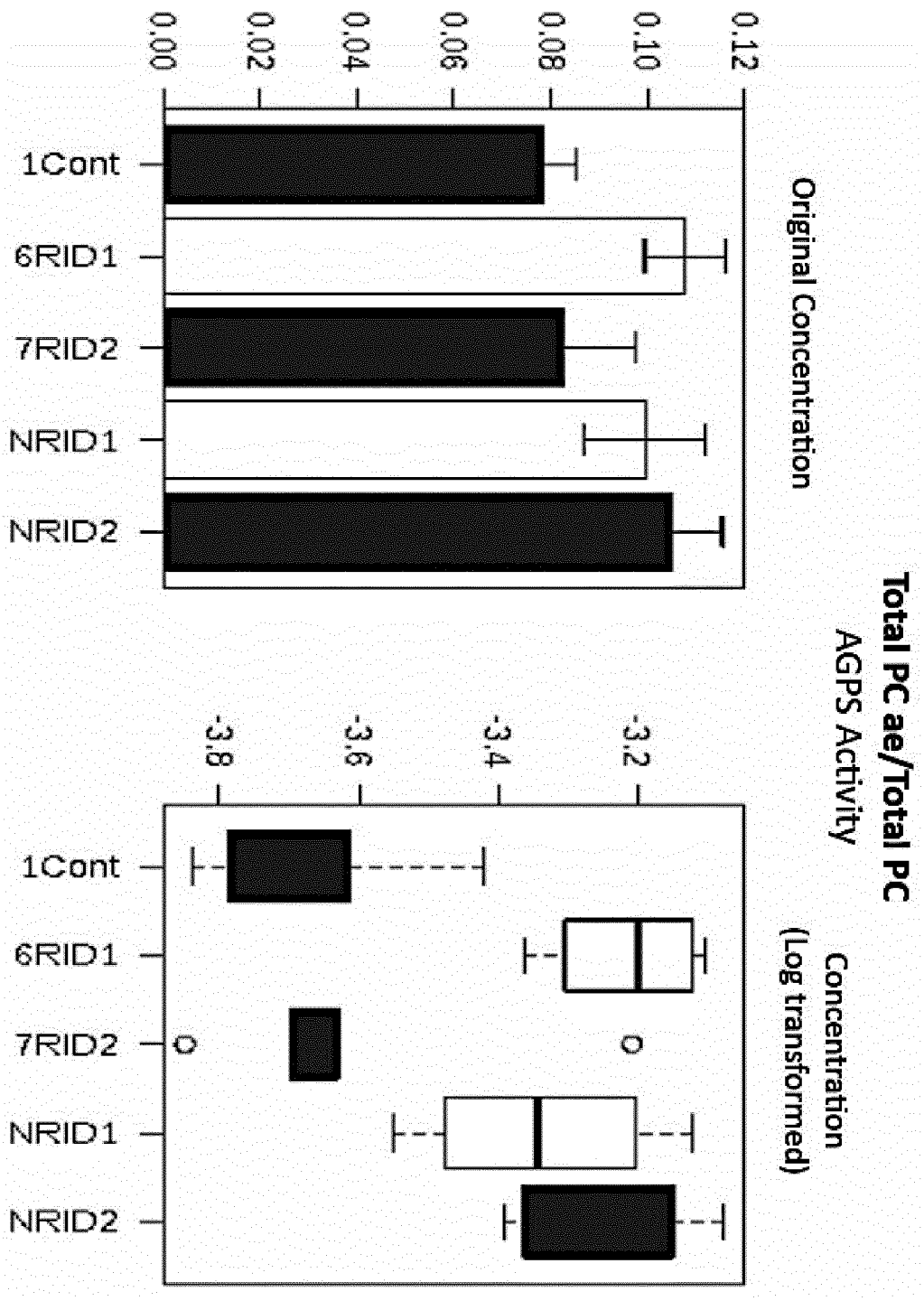

Total PC ae/Total PC
AGPS Activity
Original Concentration
0,00
0,02
0,04
0,06
0,08
0,10
0,12
1Cont
6RID1
7RID2
NRID1
NRID2
Concentration
(Log transformed)
-3,8
-3,6
-3,4
-3,2
1Cont
6RID1
7RID2
NRID1
NRID2

Figure 7C

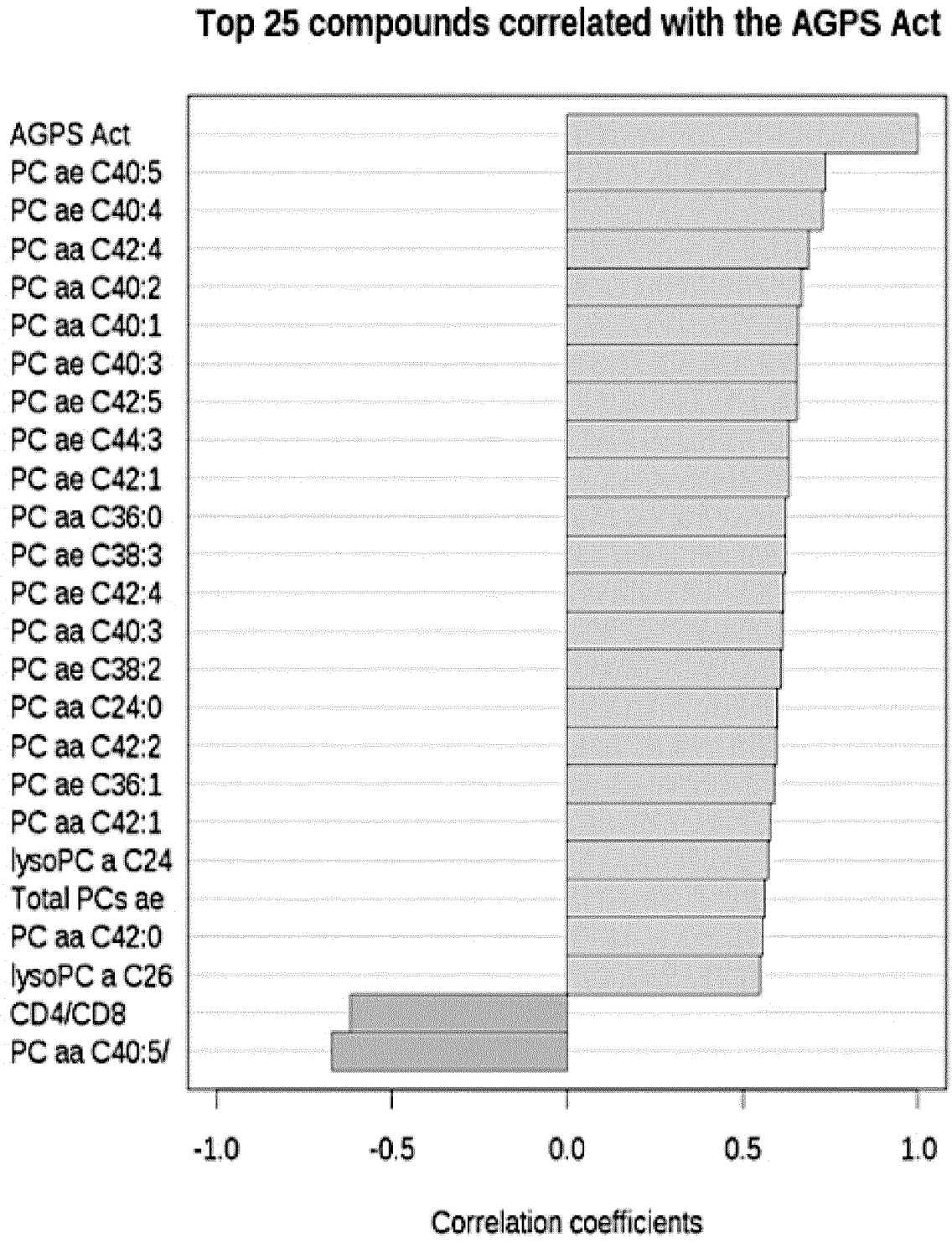

Top 25 compounds correlated with the AGPS Act
AGPS Act
PC ae C40:5
PC ae C40:4
PC aa C42:4
PC aa C40:2
PC aa C40:1
PC ae C40:3
PC ae C42:5
PC ae C44:3
PC ae C42:1
PC aa C36:0
PC ae C38:3
PC ae C42:4
PC aa C40:3
PC ae C38:2
PC aa C24:0
PC aa C42:2
PC ae C36:1
PC aa C42:1
lysoPC a C24
Total PCs ae
PC aa C42:0
lysoPC a C26
CD4/CD8
PC aa C40:5/
-1.0
-0.5
0.0
0.5
1.0
Correlation coefficients

Figure 7D

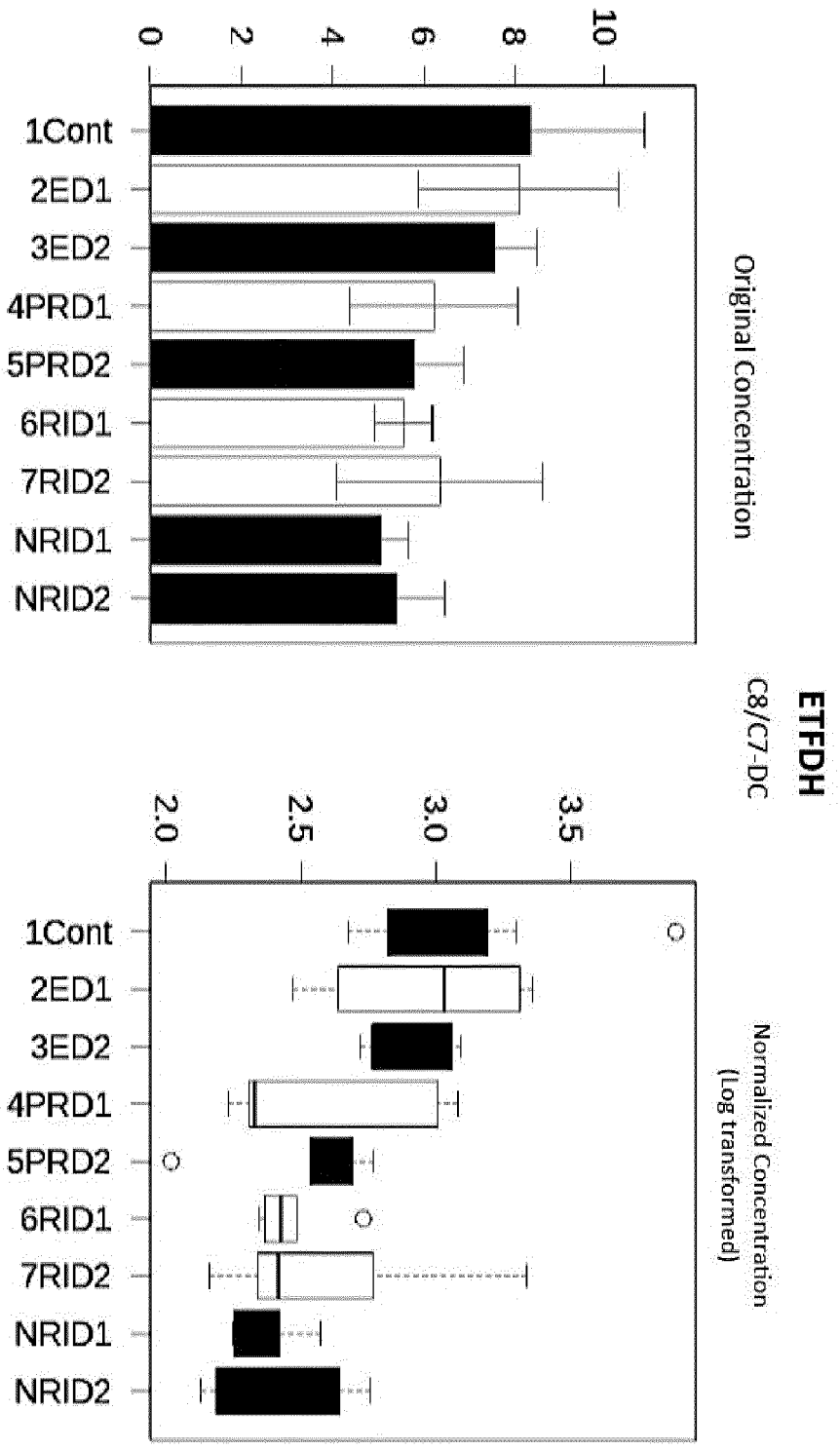

ETFDH
C8/C7-DC
Original Concentration
0
2
4
6
8
10
1Cont
2ED1
3ED2
4PRD1
5PRD2
6RID1
7RID2
NRID1
NRID2
Normalized Concentration
(Log transformed)
2.0
2.5
3.0
3.5
1Cont
2ED1
3ED2
4PRD1
5PRD2
6RID1
7RID2
NRID1
NRID2

Figure 7E

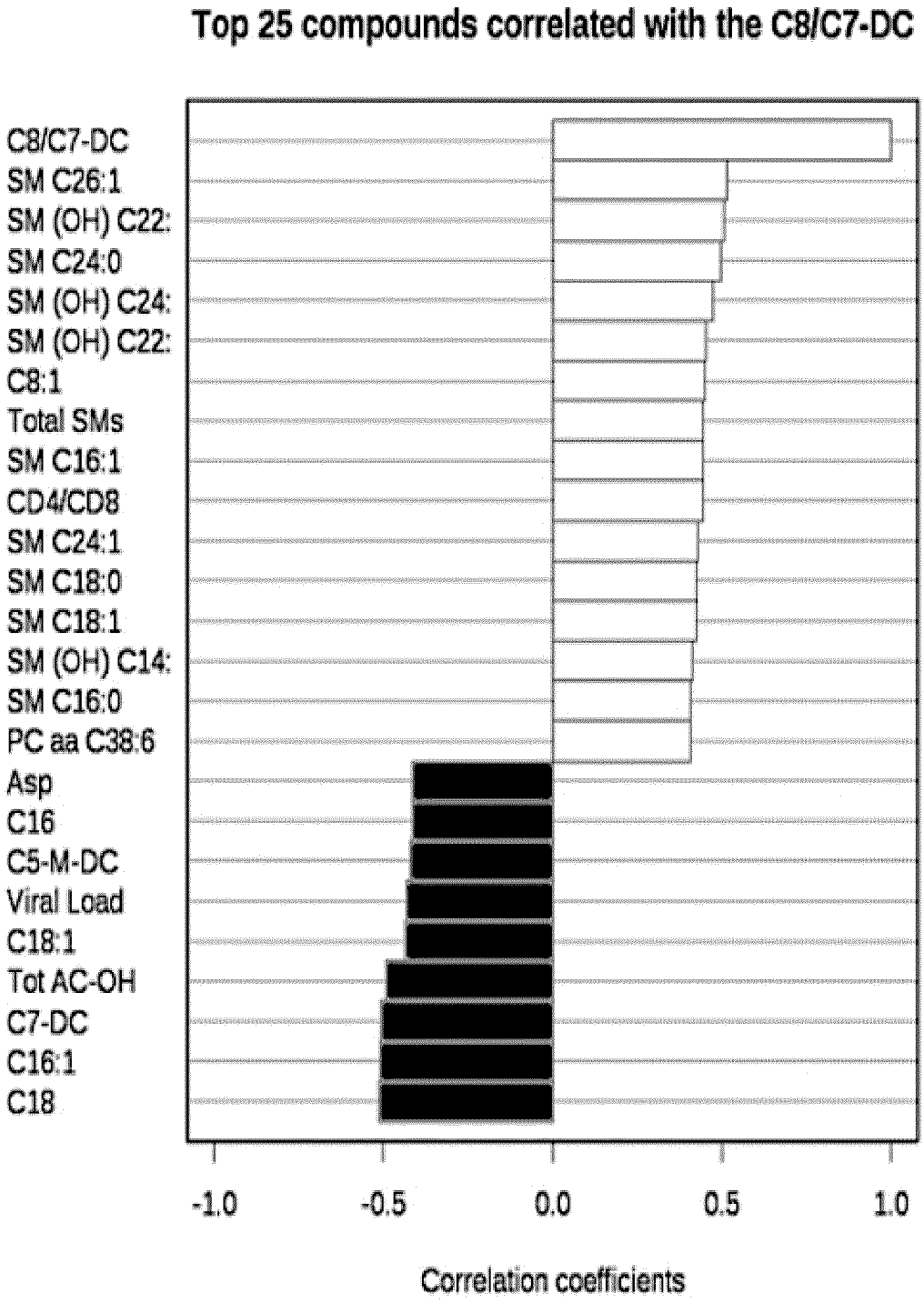

Top 25 compounds correlated with the C8/C7-DC
C8/C7-DC
SM C26:1
SM (OH) C22:
SM C24:0
SM (OH) C24:
SM (OH) C22:
C8:1
Total SMs
SM C16:1
CD4/CD8
SM C24:1
SM C18:0
SM C18:1
SM (OH) C14:
SM C16:0
PC aa C38:6
Asp
C16
C5-M-DC
Viral Load
C18:1
Tot AC-OH
C7-DC
C16:1
C18
-1.0
-0.5
0.0
0.5
1.0
Correlation coefficients

Figure 8

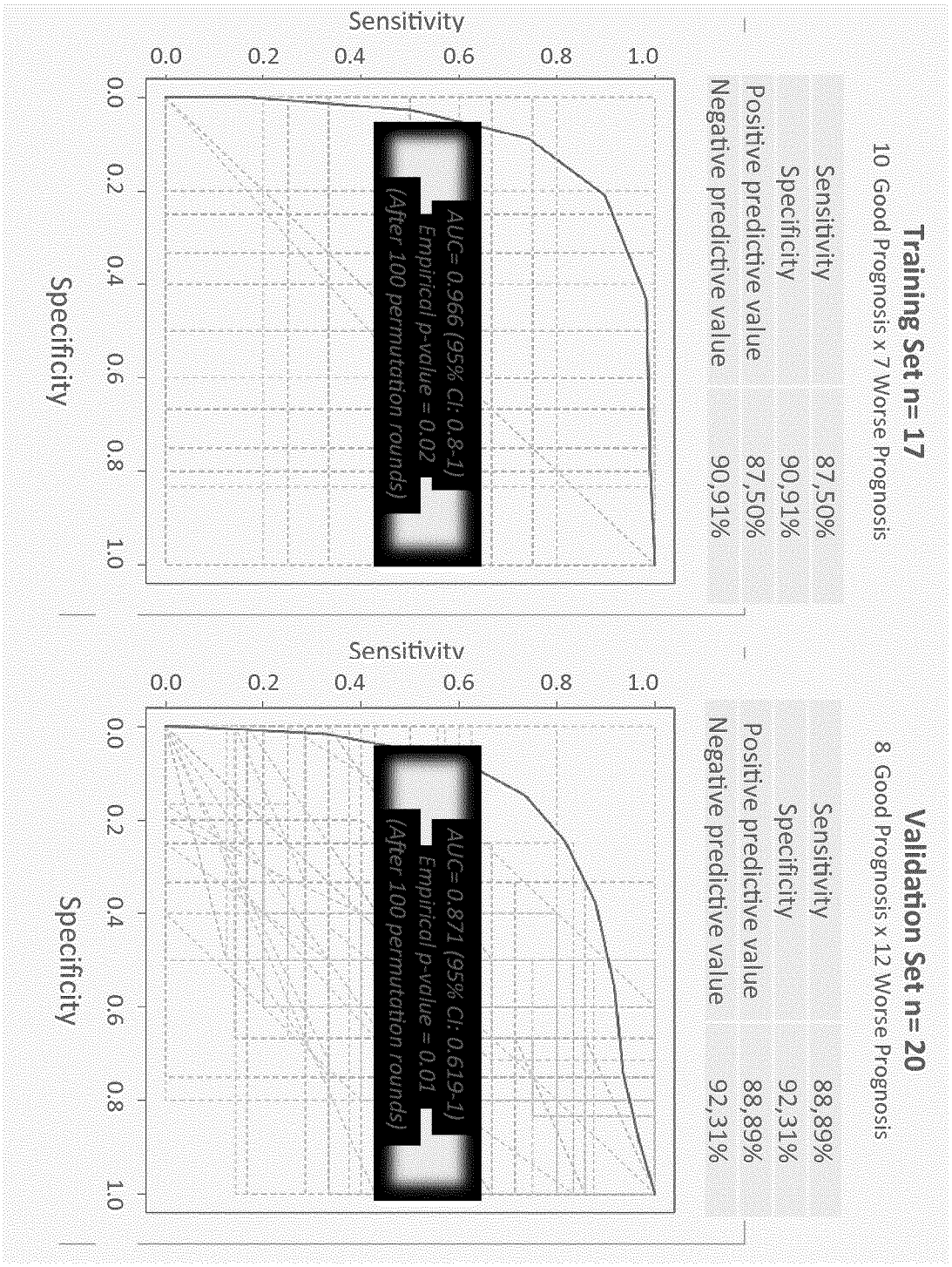

Training Set n= 17
10 Good Prognosis x 7 Worse Prognosis
Sensitivity 87,50%
Specificity 90,91%
Positive predictive value 87,50%
Negative predictive value 90,91%
Sensitivity
Specificity
AUC= 0.966 (95% CI: 0.8-1)
Empirical p-value = 0.02
(After 100 permutation rounds)
Validation Set n= 20
8 Good Prognosis x 12 Worse Prognosis
Sensitivity 88,89%
Specificity 92,31%
Positive predictive value 88,89%
Negative predictive value 92,31%
Sensitivity
Specificity
AUC= 0.871 (95% CI: 0.619-1)
Empirical p-value = 0.01
(After 100 permutation rounds)

Figure 9

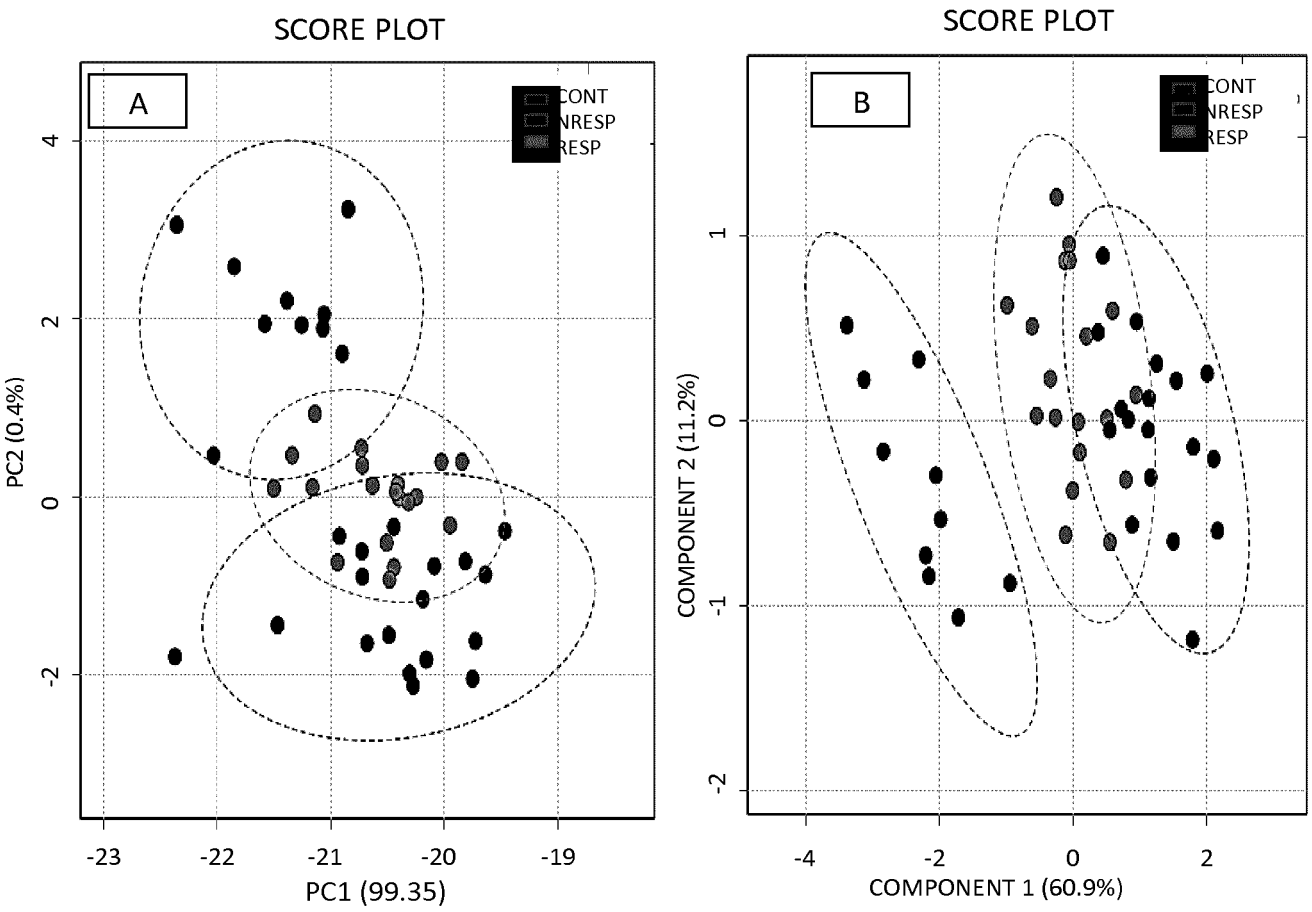

SCORE PLOT
A
CONT
NRESP
RESP
PC2 (0.4%)
4
2
0
-2
-23
-22
-21
-20
-19
PC1 (99.35)
SCORE PLOT
B
CONT
NRESP
RESP
COMPONENT 2 (11.2%)
1
0
-1
-2
-4
-2
0
2
COMPONENT 1 (60.9%)

Figure 10A

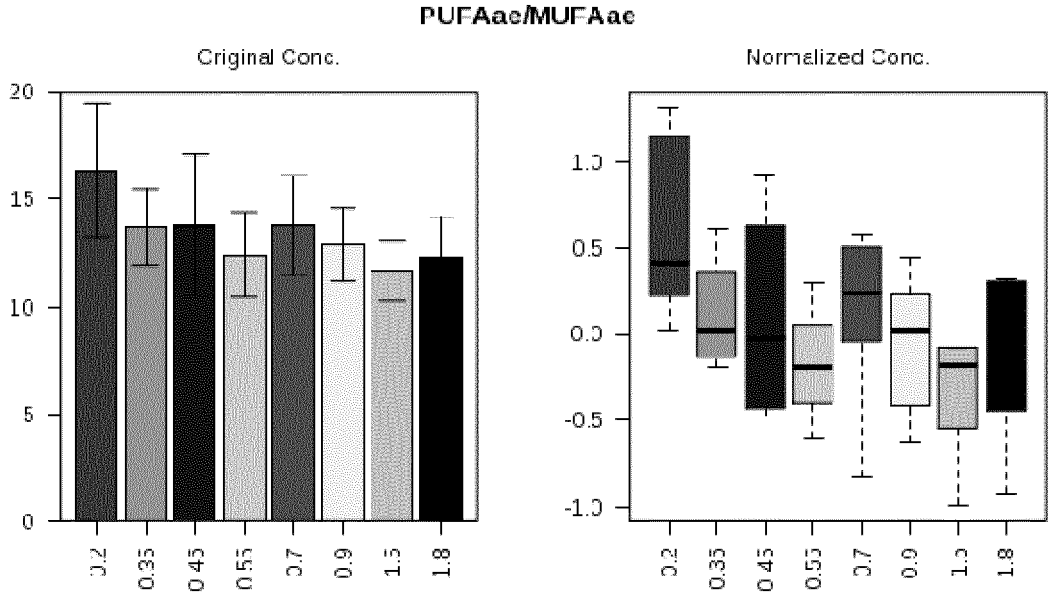


Figure 10B

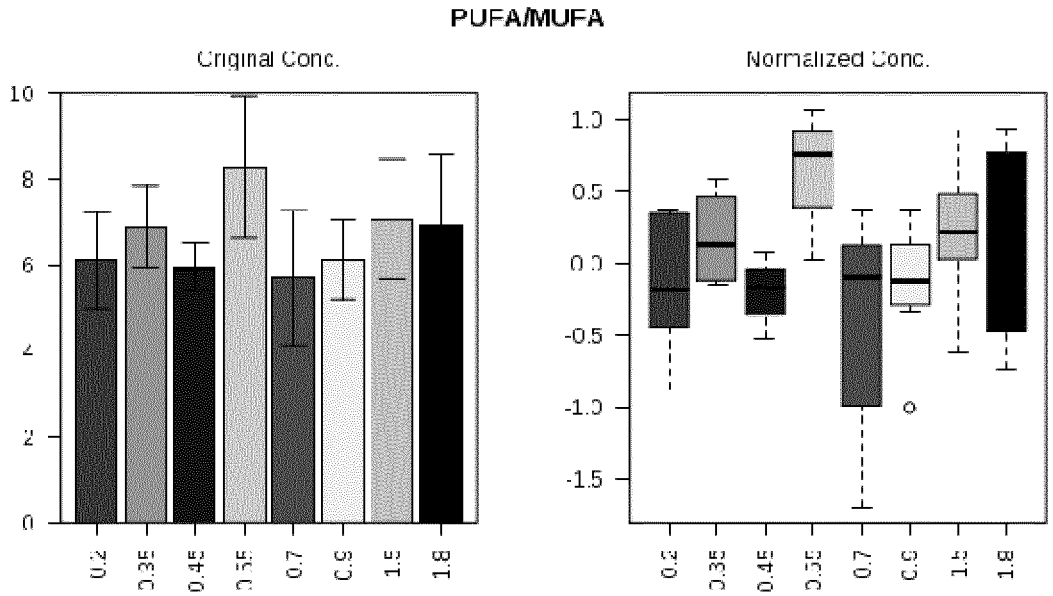


Figure 11A

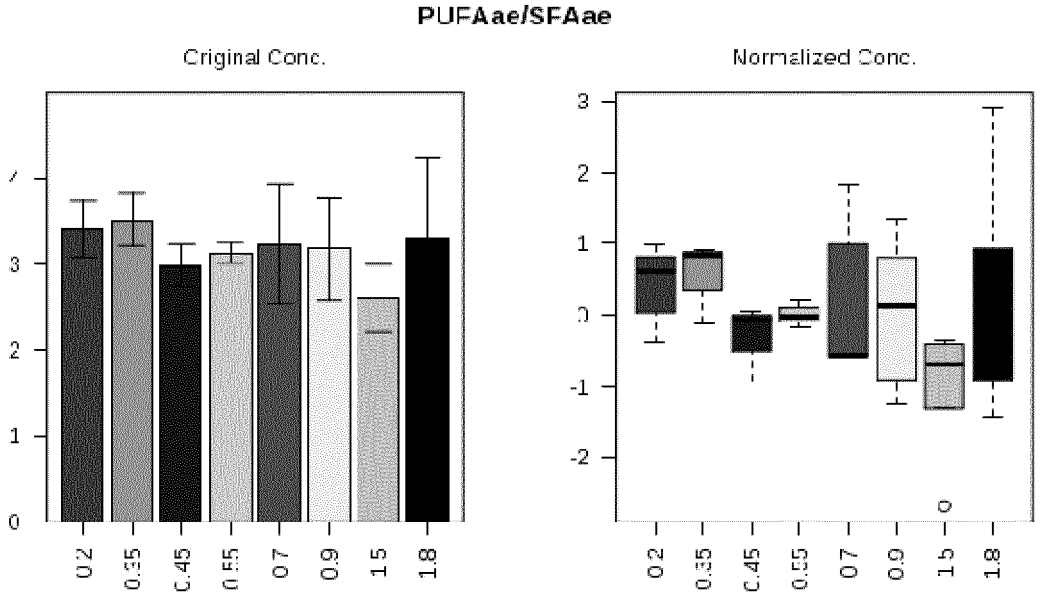


Figure 11B

