Supplementary Material for:

Metabolic profiling comparison of human pancreatic ductal epithelial cells and three pancreatic cancer cell lines using NMR based metabonomics.

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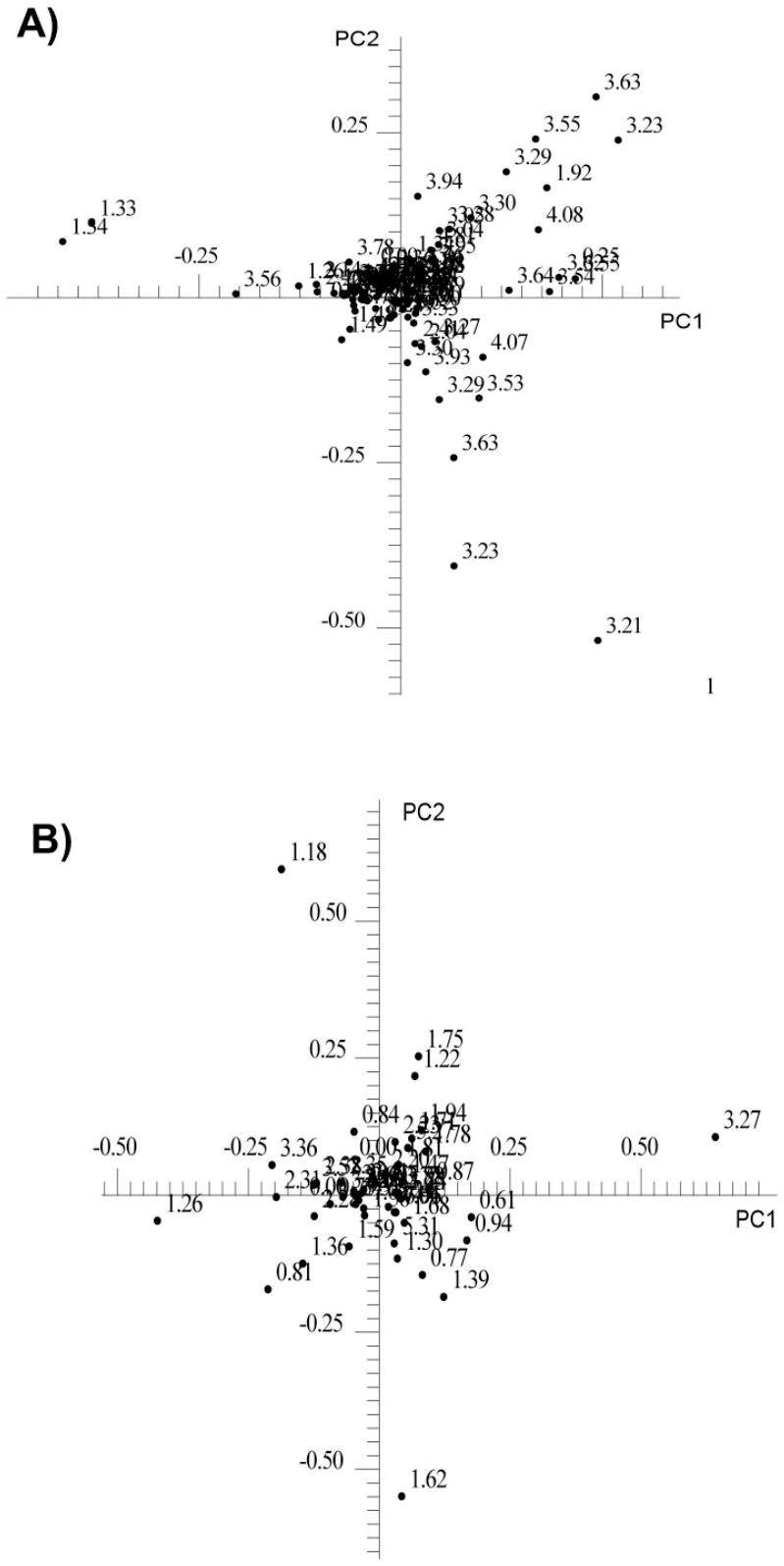
Contents:

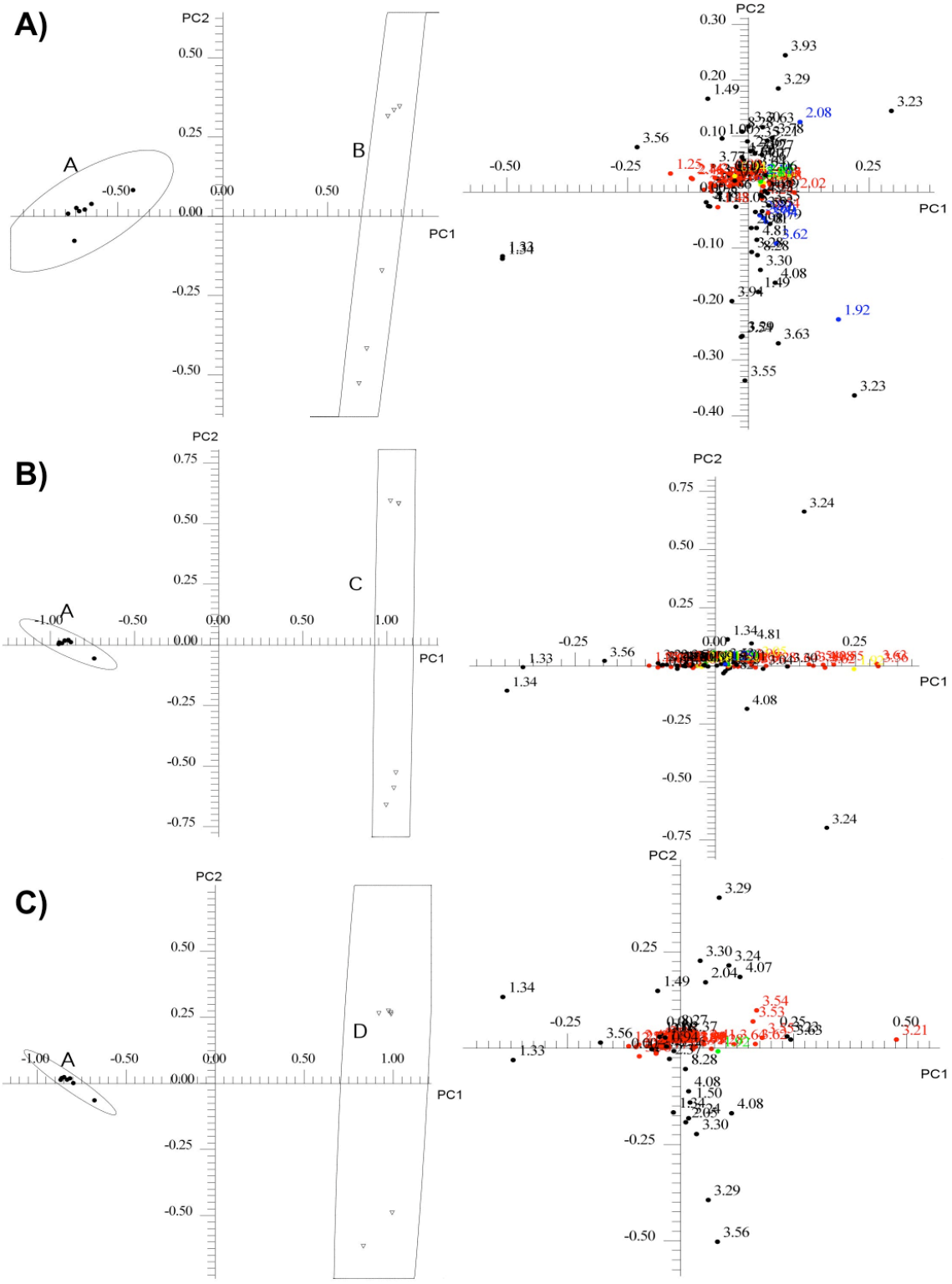
Supplemental Figure 1. (A) Two-dimensional PC1 versus PC2 loadings plot corresponding to the scores plot of hydrophilic cell extract data in Fig 3A. (B) Two-dimensional PC1 versus PC2 loadings plot corresponding to the scores plot of lipophilic cell extract data in Fig 3B.

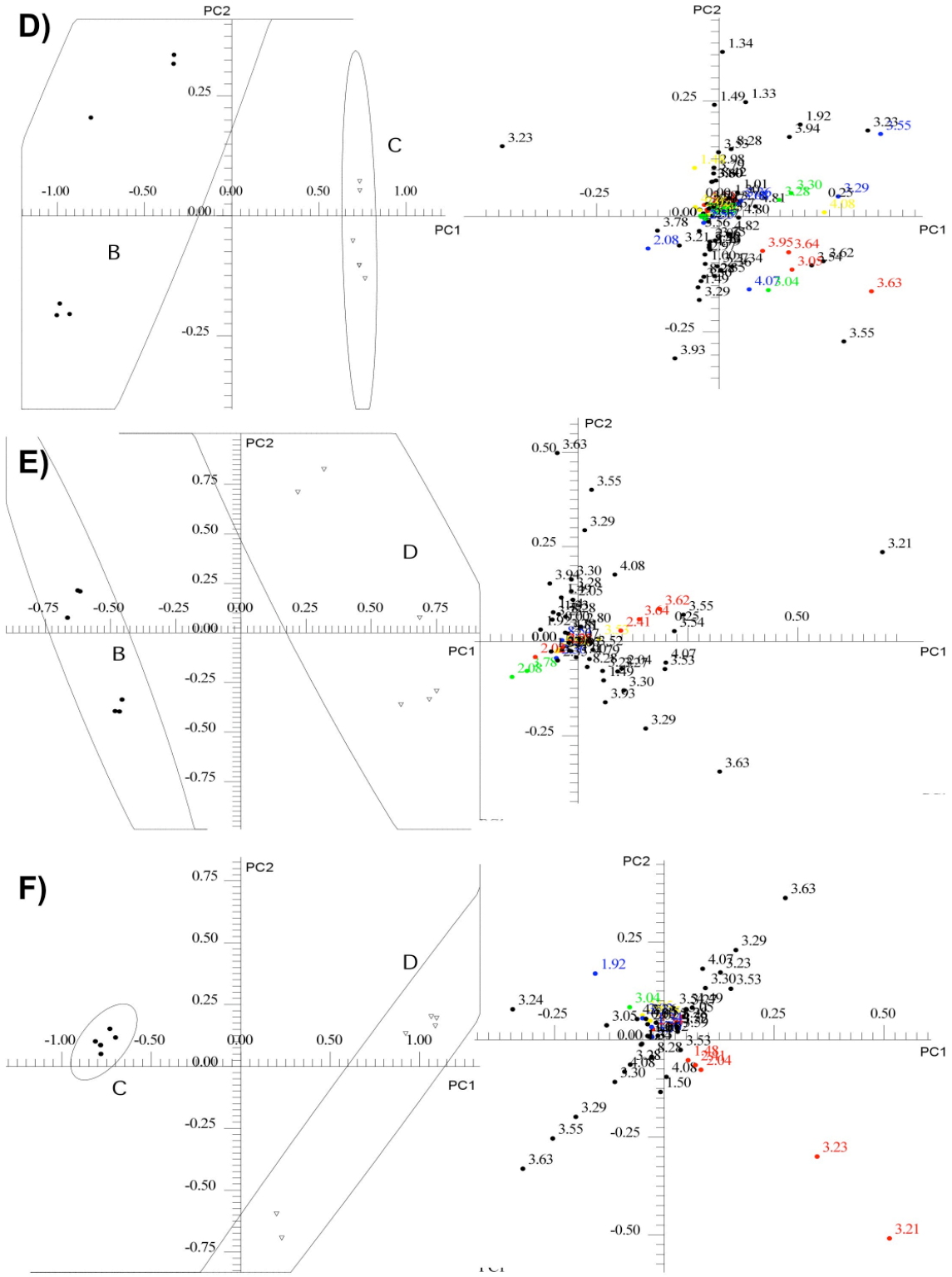
Supplemental Figure 2. Two-dimensional PC1 versus PC2 scores plot and the loadings plot comparing hydrophilic extracts of A)H6C7 and Miapaca-2, B)H6C7 and Panc-1, C)H6C7 and AsPC-1, D)Miapaca-2 and Panc-1, E)Miapaca-2 and AsPC-1, F)Panc-1 and AsPC-1.

Supplemental Figure 3. Two-dimensional PC1 versus PC2 scores plot and the loadings plot comparing lipophilic extracts of A)H6C7 and Miapaca-2, B)H6C7 and Panc-1, C)H6C7 and AsPC-1, D)Miapaca-2 and Panc-1, E)Miapaca-2 and AsPC-1, F)Panc-1 and AsPC-1.

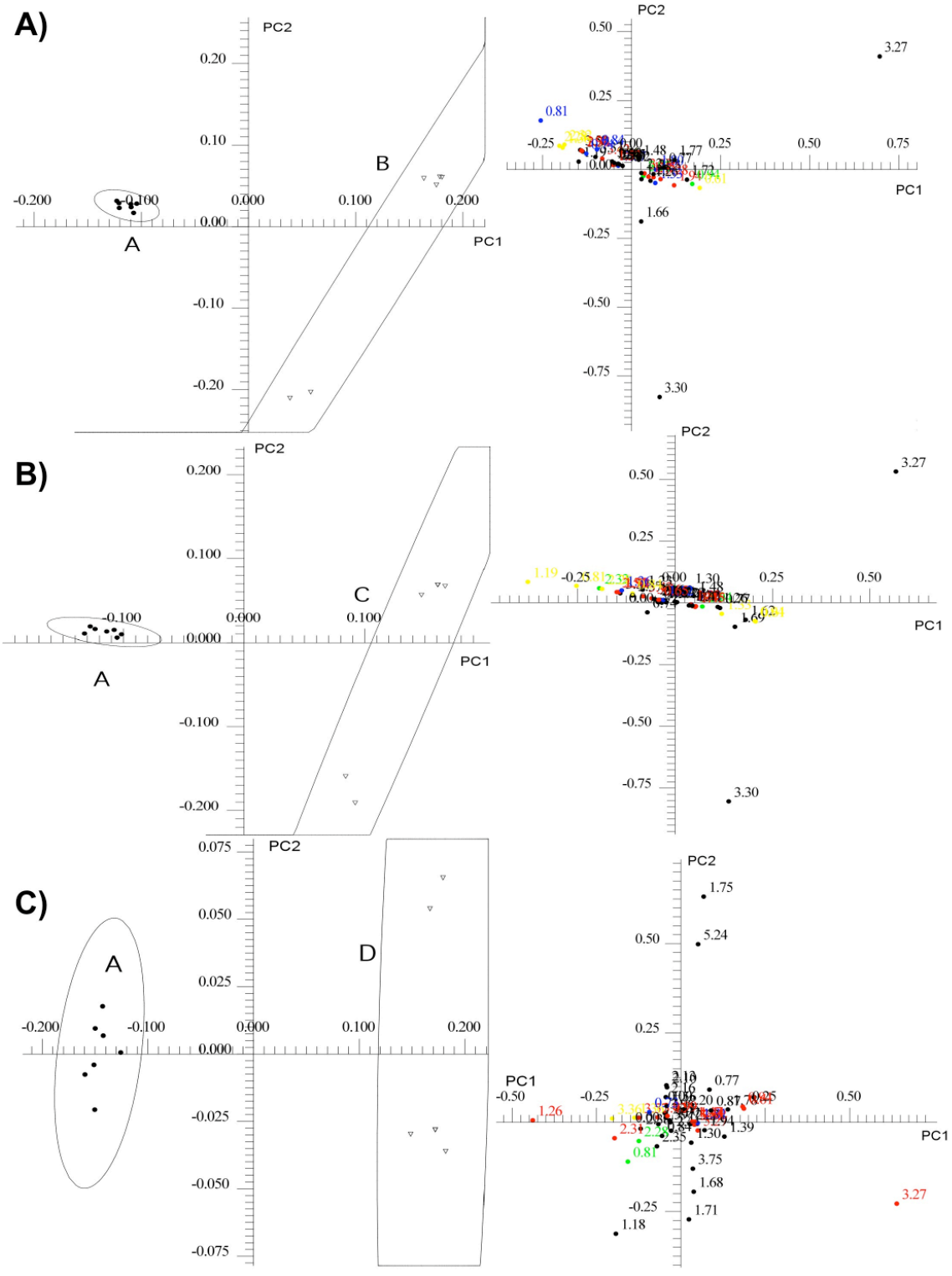


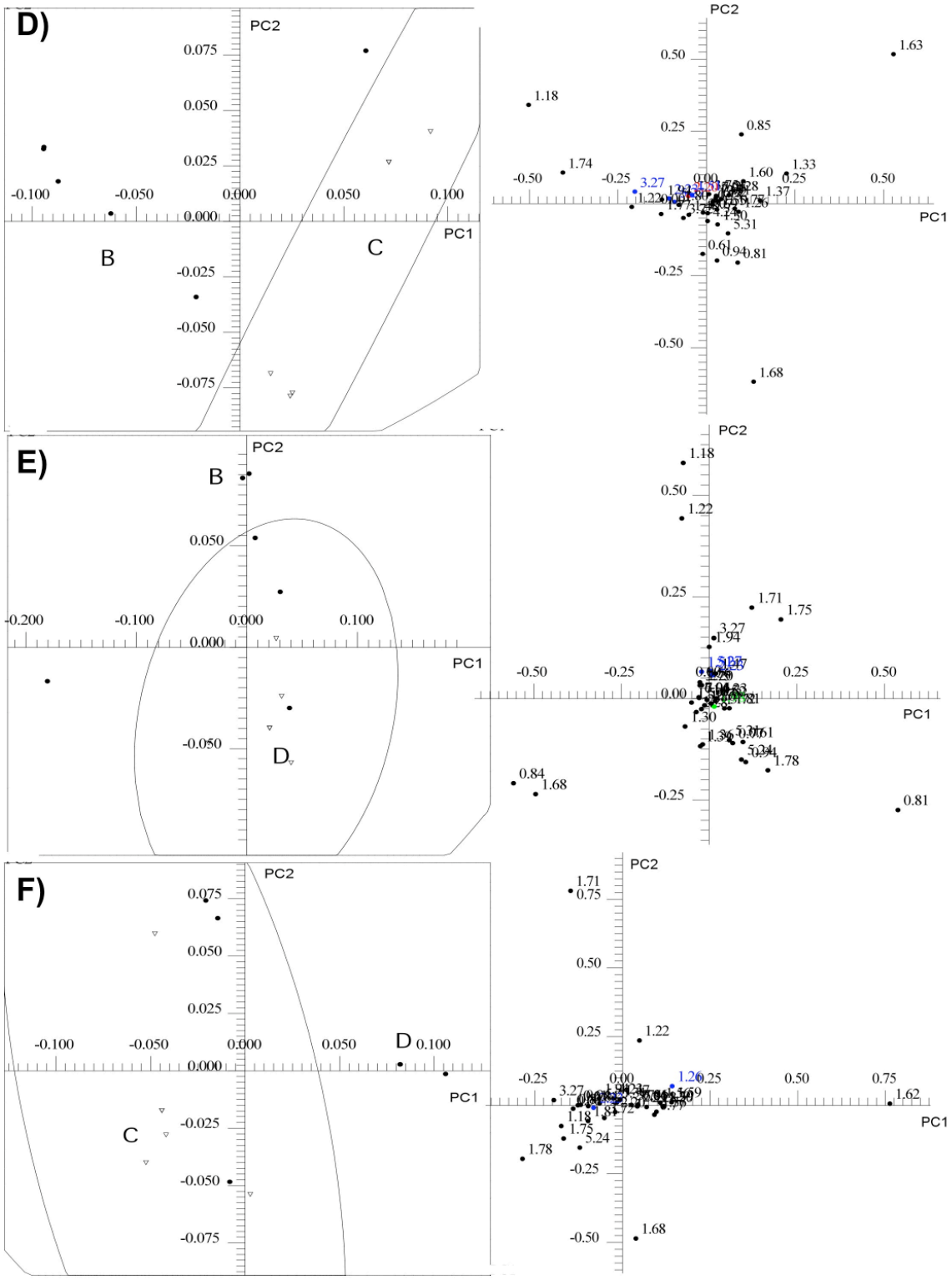
Supplemental Figure 1. (A) Two-dimensional PC1 versus PC2 loadings plot corresponding to the scores plot of hydrophilic cell extract data in Fig 3A. (B) Two-dimensional PC1 versus PC2 loadings plot corresponding to the scores plot of lipophilic cell extract data in Fig 3B.


A)
PC2
PC1
A
B
B)
C
C)
D



Supplemental Figure 2. Two-dimensional PC1 versus PC2 scores plot and the loadings plot comparing hydrophilic extracts of A)H6C7 and Miapaca-2, B)H6C7 and Panc-1, C)H6C7 and AsPC-1, D)Miapaca-2 and Panc-1, E)Miapaca-2 and AsPC-1, F)Panc-1 and AsPC-1. In the scores plot, the 95% confidence interval for the two clusters of data points were indicated with oval lines. The Bonferroni-corrected *p*-values from 0.005 ppm buckets for hydrophilic cell extracts were determined for each comparison and listed in Table 2 The loading plots are color-coded according to bucket *p*-values: Black (>α-value), Blue (α-value - 10^{-5}), Green (10^{-5}- 10^{-6}), Yellow (10^{-6} - 10^{-7}), Red (10^{-7}- 0).


A)
PC2
PC1
A
B
B)
C
C)
D



Supplemental Figure 3. Two-dimensional PC1 versus PC2 scores plot and the loadings plot comparing lipophilic extracts of A)H6C7 and Miapaca-2, B)H6C7 and Panc-1, C)H6C7 and AsPC-1, D)Miapaca-2 and Panc-1, E)Miapaca-2 and AsPC-1, F)Panc-1 and AsPC-1. In the scores plot, the 95% confidence interval for the two clusters of data points were indicated with oval lines. The Bonferroni-corrected *p*-values from 0.03 ppm buckets for lipophilic cell extracts were determined for each comparison and listed in Table 2. The loading plots are color-coded according to bucket *p*-values: Black (>α-value), Blue (α-value - 10^{-5}), Green (10^{-5}- 10^{-6}), Yellow (10^{-6} - 10^{-7}), Red (10^{-7}- 0).