## Random Forest Confusion Matrix

**Predicted Group**

| Actual Group | II | III | IV | Class Error |
|---|---|---|---|---|
| II | 14 | 4 | 0 | 0.22 |
| III | 5 | 6 | 7 | 0.67 |
| IV | 2 | 2 | 29 | 0.12 |
| Predictive accuracy = 71% | | | | |

Figure S1

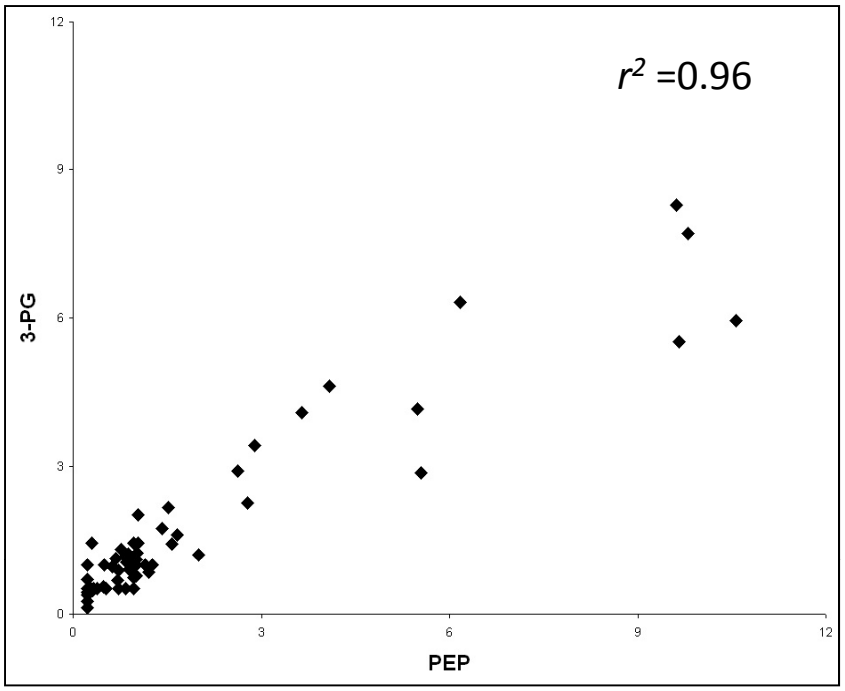


Figure S2

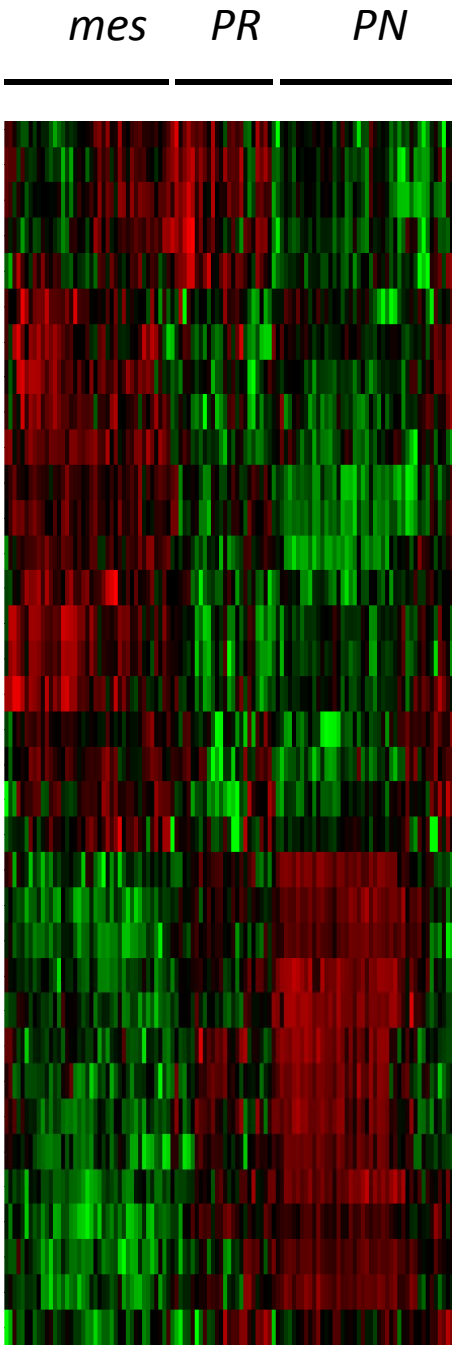


Figure S3

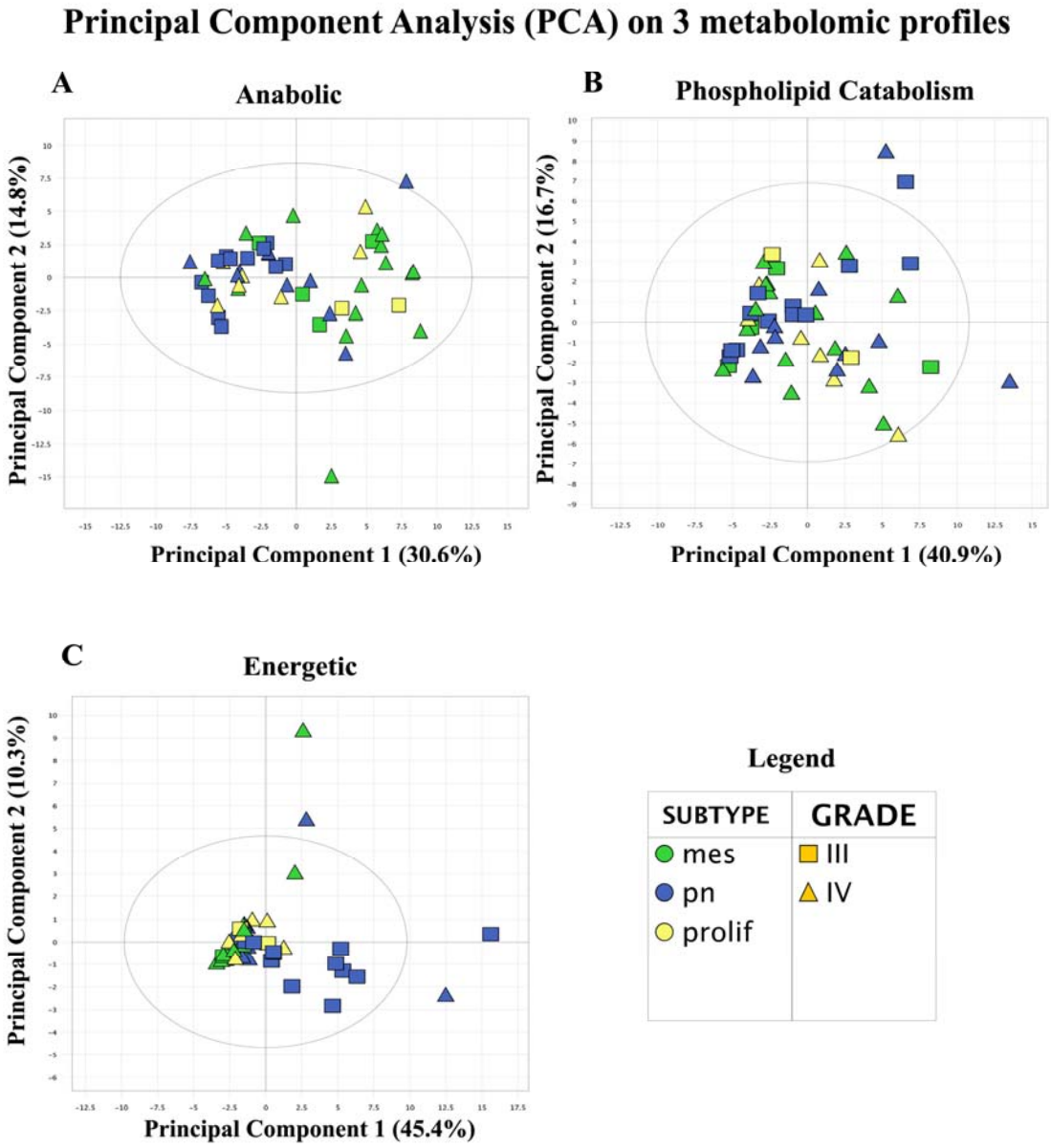
Principal Component Analysis (PCA) on 3 metabolomic profiles
A
Anabolic
Principal Component 2 (14.8%)
Principal Component 1 (30.6%)
B
Phospholipid Catabolism
Principal Component 2 (16.7%)
Principal Component 1 (40.9%)
C
Energetic
Principal Component 2 (10.3%)
Principal Component 1 (45.4%)
Legend
SUBTYPE
mes
pn
prolif
GRADE
III
IV

Figure S4