# Data Not Shown - Manuscript Sentences

## Sample Composition

Of the 62 samples run, 33 (53%) were arterial and 29 (47%) were venous.

## PGD Grade Distribution

Of the 62 patients, 36 (58%) had no PGD, 1 (2%) had mild PGD, 17 (27%) had moderate PGD, and 8 (13%) had severe PGD.

## Sample Processing Times

Sample processing times ranged from 0.15 to 4.75 hours (mean = 0.95 hours).

## Feature Counts

A total of 23692 metabolomic features were detected across both chromatography methods (13072 HILIC and 10620 C18 features). After filtering based on QC measures, 16283 features remained (7907 HILIC and 8376 C18 features).

## Volcano Plot Results

Further analysis identified 1071 significantly different untargeted metabolite features between groups, among which 506 metabolites were at least 1.5-fold higher in the PGD group, while 94 metabolites were at least 1.5-fold lower.

## Mummichog Parameters