

COMPARING 3 BRANDS OF ASPIRIN PILLS •

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Using dataset from: LC-MS/MS in the Clinical Laboratory – Where to From Here?

by Stefan KG Greve and Ravinder J Singh and which can be found here:
<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3052391/>

Intro



Background and Dataset

- Machine generated dataset analyzing the chemical make-up and intensities of three brands of aspirin pills
- Dataset consists of:
 - 3 pills from 3 different brands of aspirin (Bayer, PV, and Walgreens)
 - Dataset consists of 63 tsv files grouping the pills by brand, peak of intensity, replicant, and aliquot
 - There are 3 aliquots for each replicant, 3 replicants for each peak, and 7 peaks for each brand in the dataset
 - Peak: time when the intensity of each pill is at its highest, usually when a chemical is released from the pill, usually at artificially timed intervals
 - Replicant: replicas of the same pill; 3 replicas of 3 different brands have been tested
 - Aliquots: Series of measurements within a timeframe of less than a second

Intro

Objective and Assumptions

- Objective is to test the null hypothesis that the 3 brands of aspirin are the same with a 95% confidence interval
 - Plan is to measure the Area Under a Peak (AUP) for each aliquot of each replicant
 - Next, run various ANOVA analyses to compare the AUPs between brands for each peak to confirm or deny the null hypothesis
- Assumptions:
 - Data was gathered using a standardized process, since it was machine generated
 - There is still some possibility for error within the process utilized to attain the data
 - Thus, missing data will be removed, and statistical tests will be run with and without outliers.

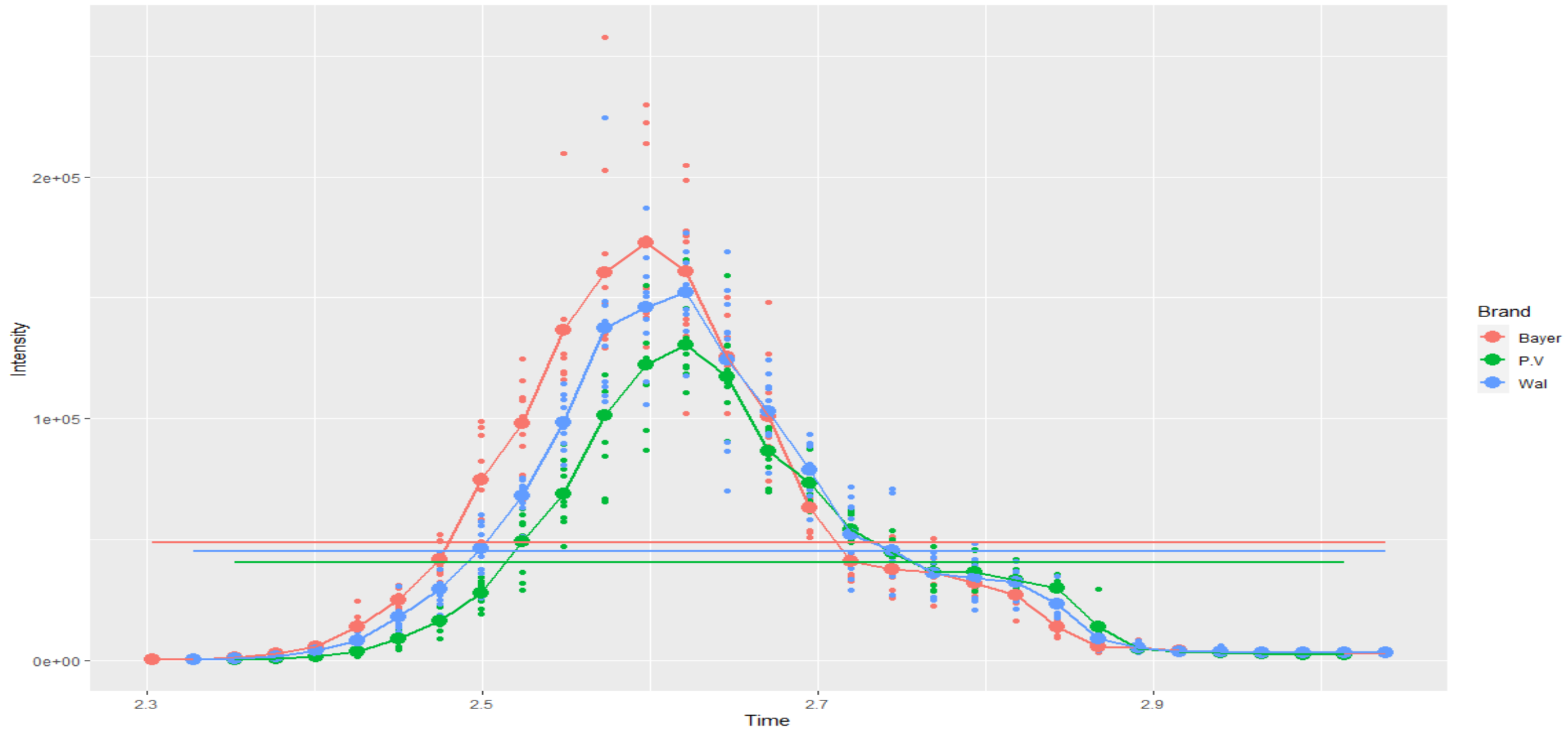
Exploratory Analysis

Dataset Summary

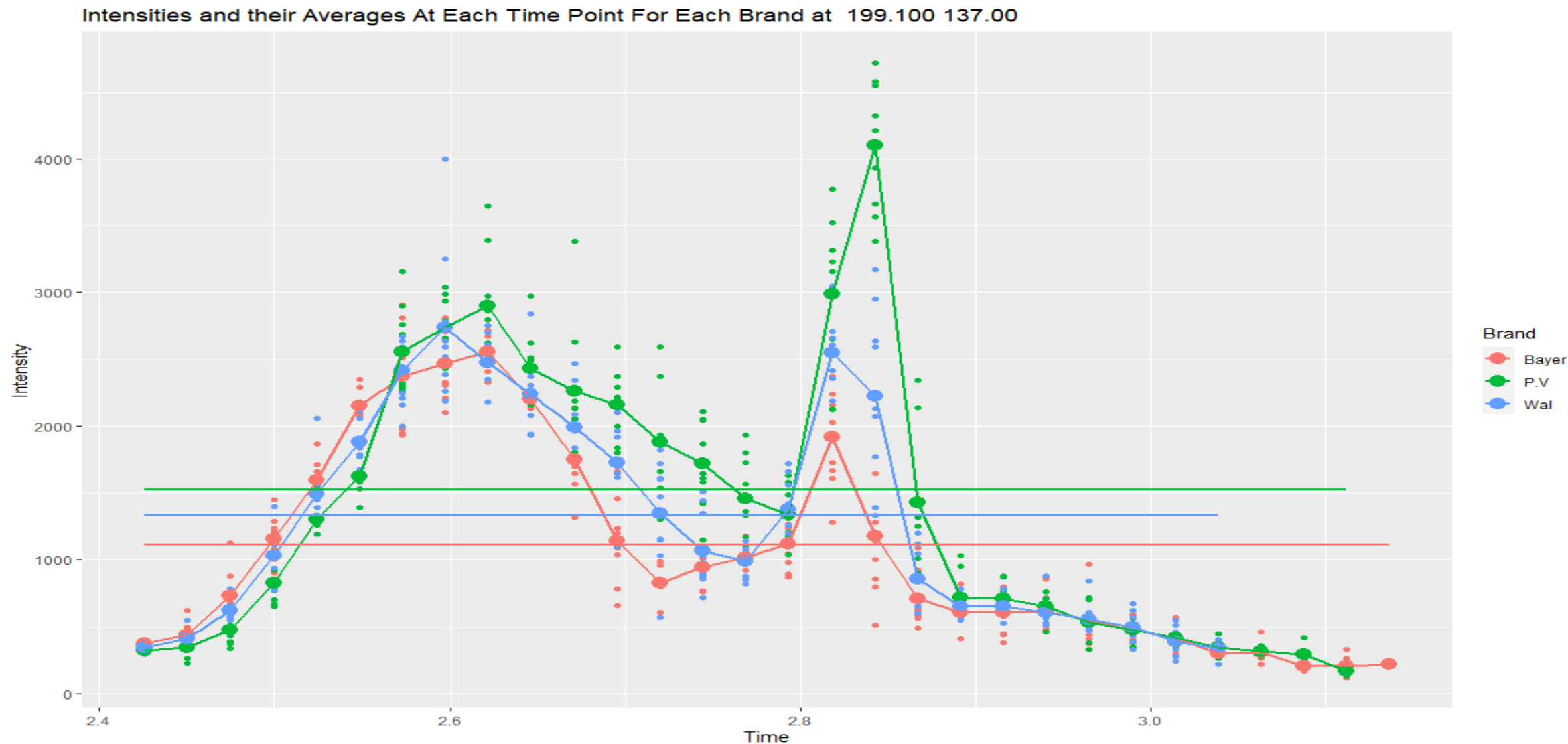
##	Brand	Peak	Replicant	Aliquot
##	Length:4798	Length:4798	Min. :1.00	Min. :1.000
##	Class :character	Class :character	1st Qu.:1.00	1st Qu.:1.000
##	Mode :character	Mode :character	Median :2.00	Median :2.000
##			Mean :1.99	Mean :2.003
##			3rd Qu.:3.00	3rd Qu.:3.000
##			Max. :3.00	Max. :3.000
##	Time	Intensity		
##	Min. :2.303	Min. : 10		
##	1st Qu.:2.548	1st Qu.: 270		
##	Median :2.720	Median : 785		
##	Mean :2.717	Mean : 10071		
##	3rd Qu.:2.867	3rd Qu.: 2590		
##	Max. :3.161	Max. :257870		

Exploratory Analysis

Intensities and their Averages At Each Time Point For Each Brand at 136.5 92.90

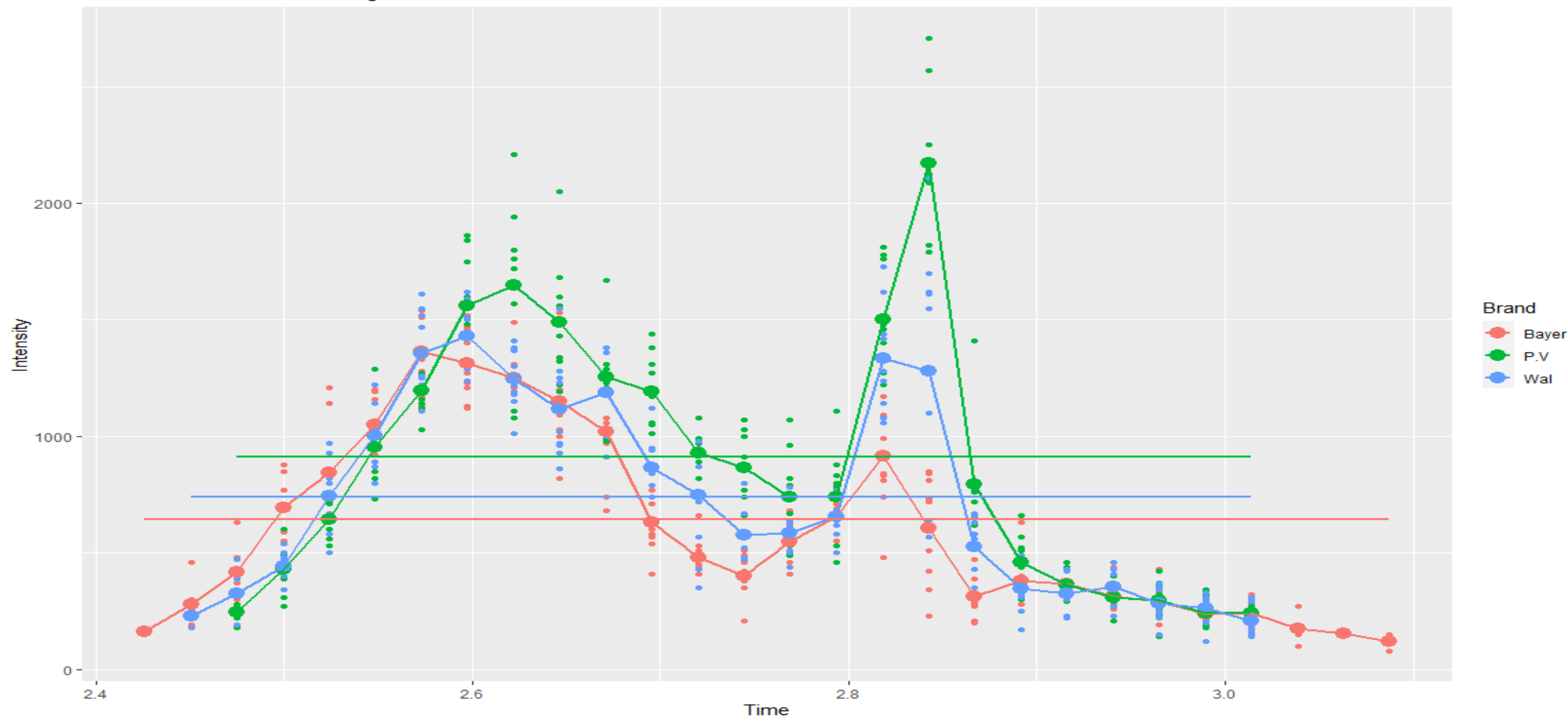


Exploratory Analysis

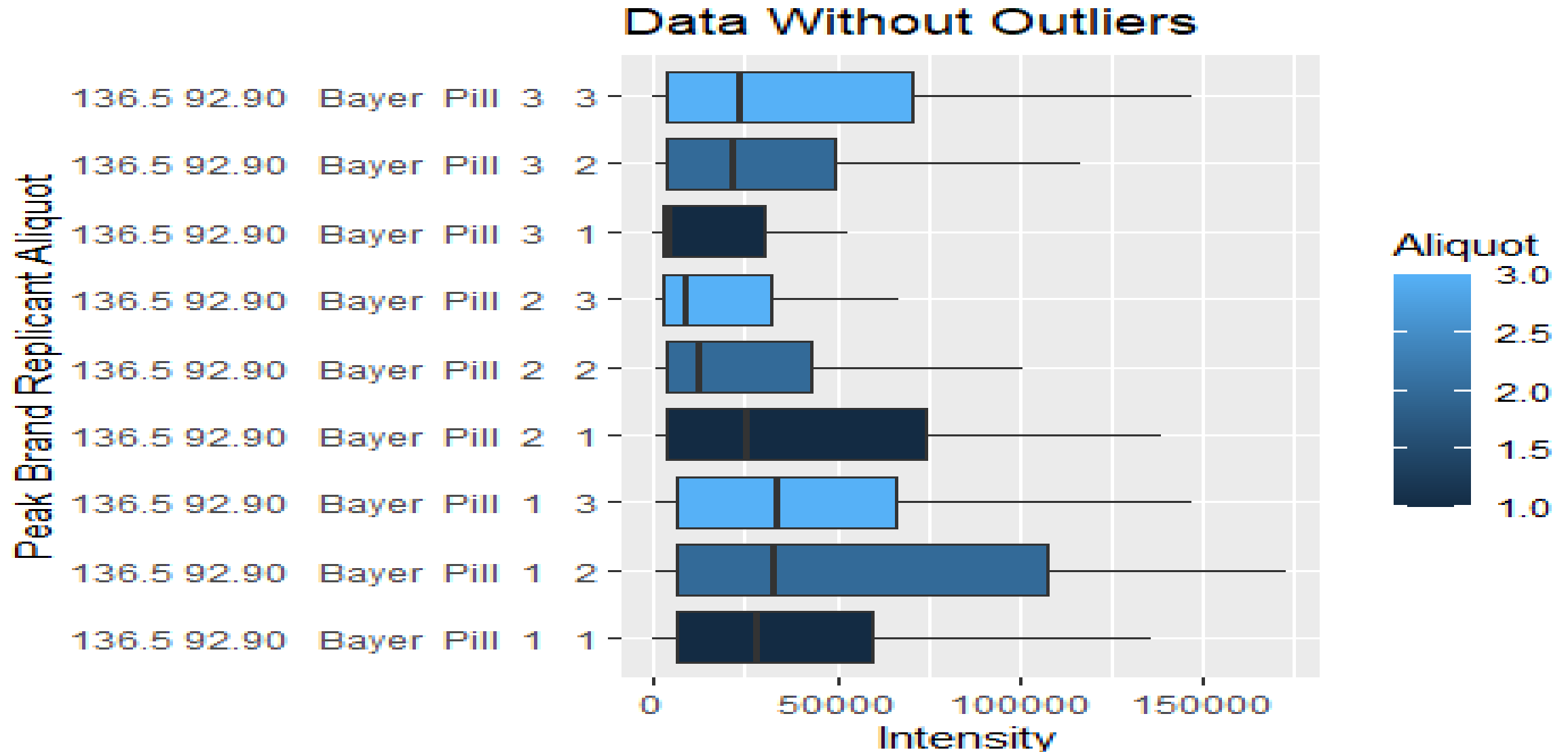


Exploratory Analysis

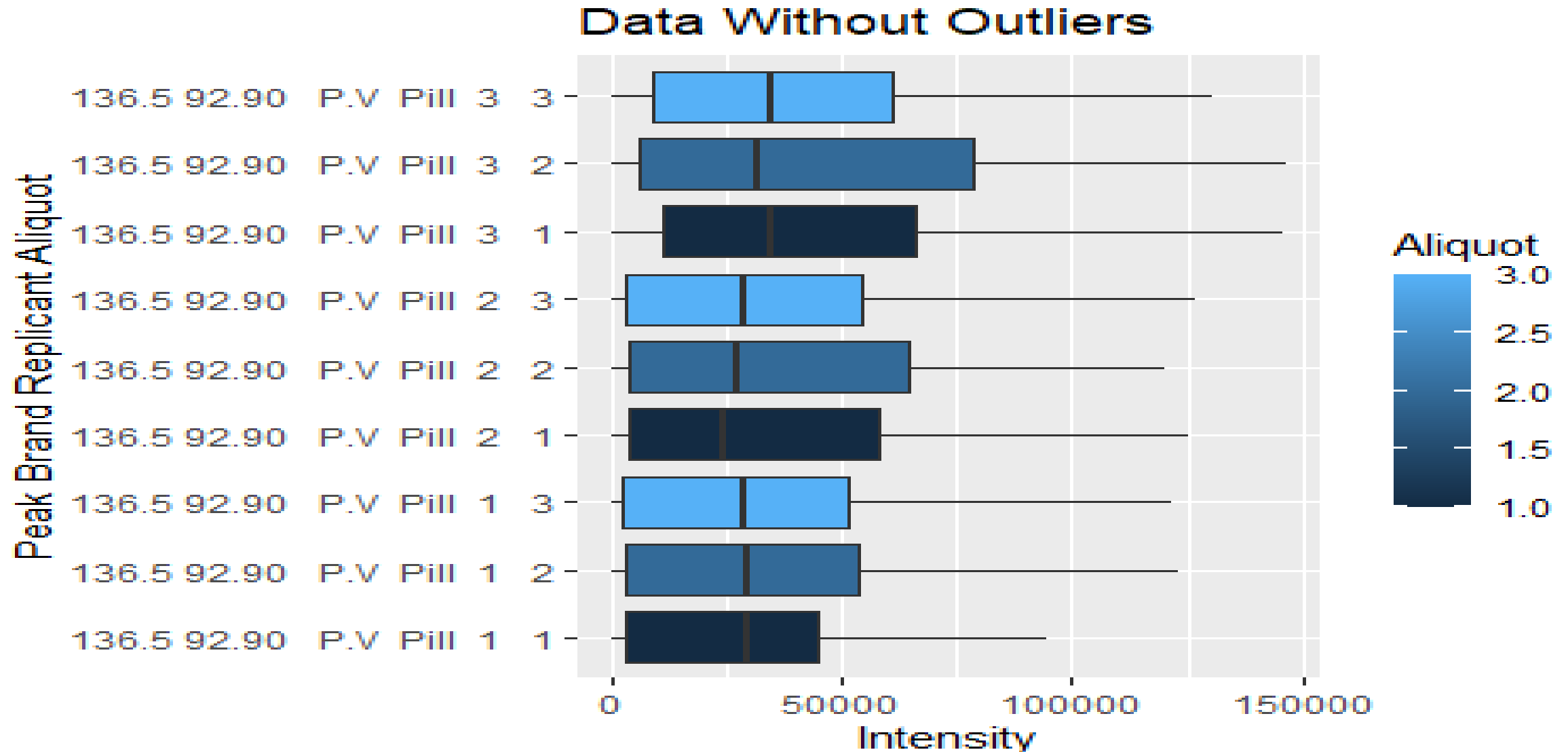
Intensities and their Averages At Each Time Point For Each Brand at 199.10 91.90



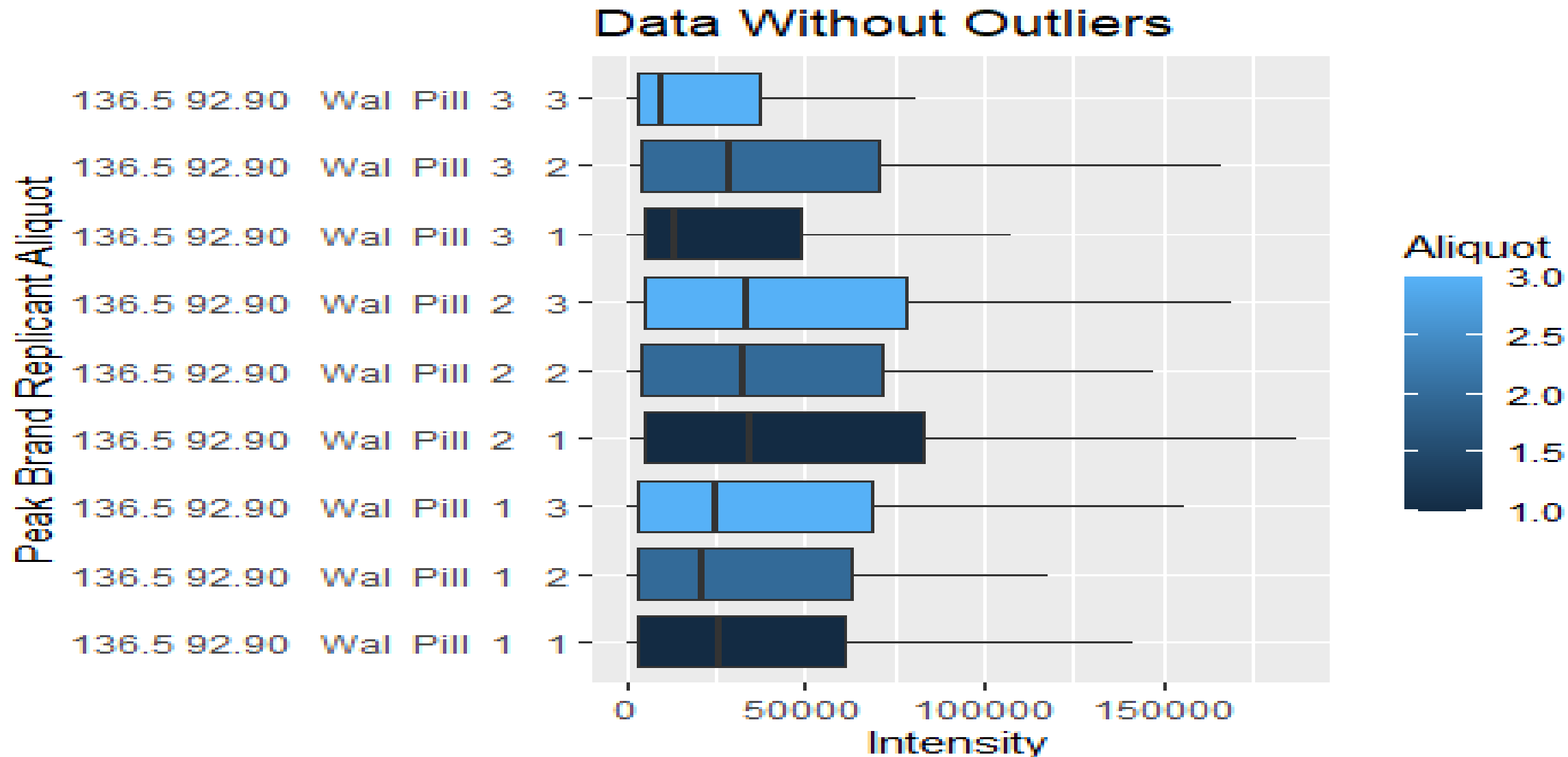
Exploratory Analysis



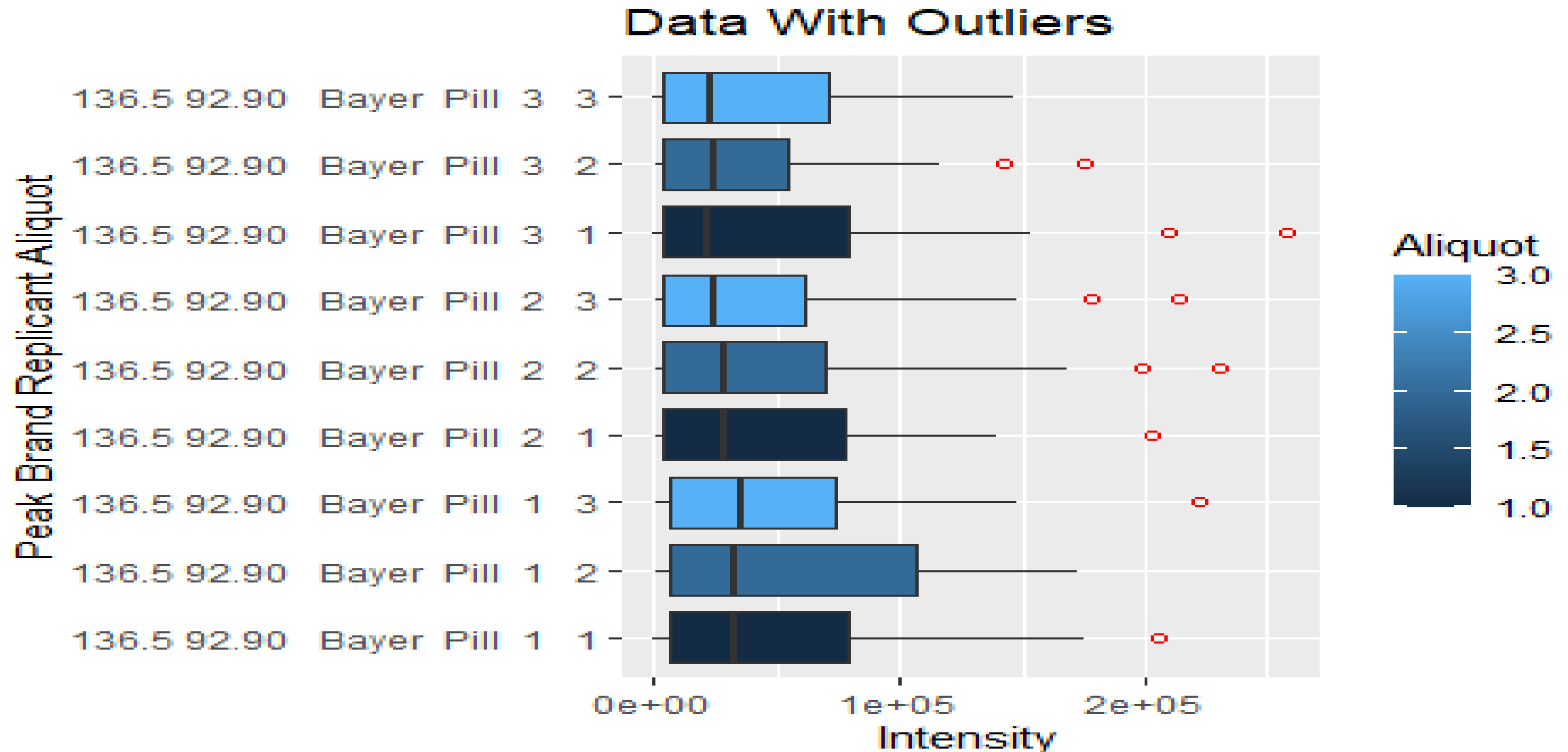
Exploratory Analysis



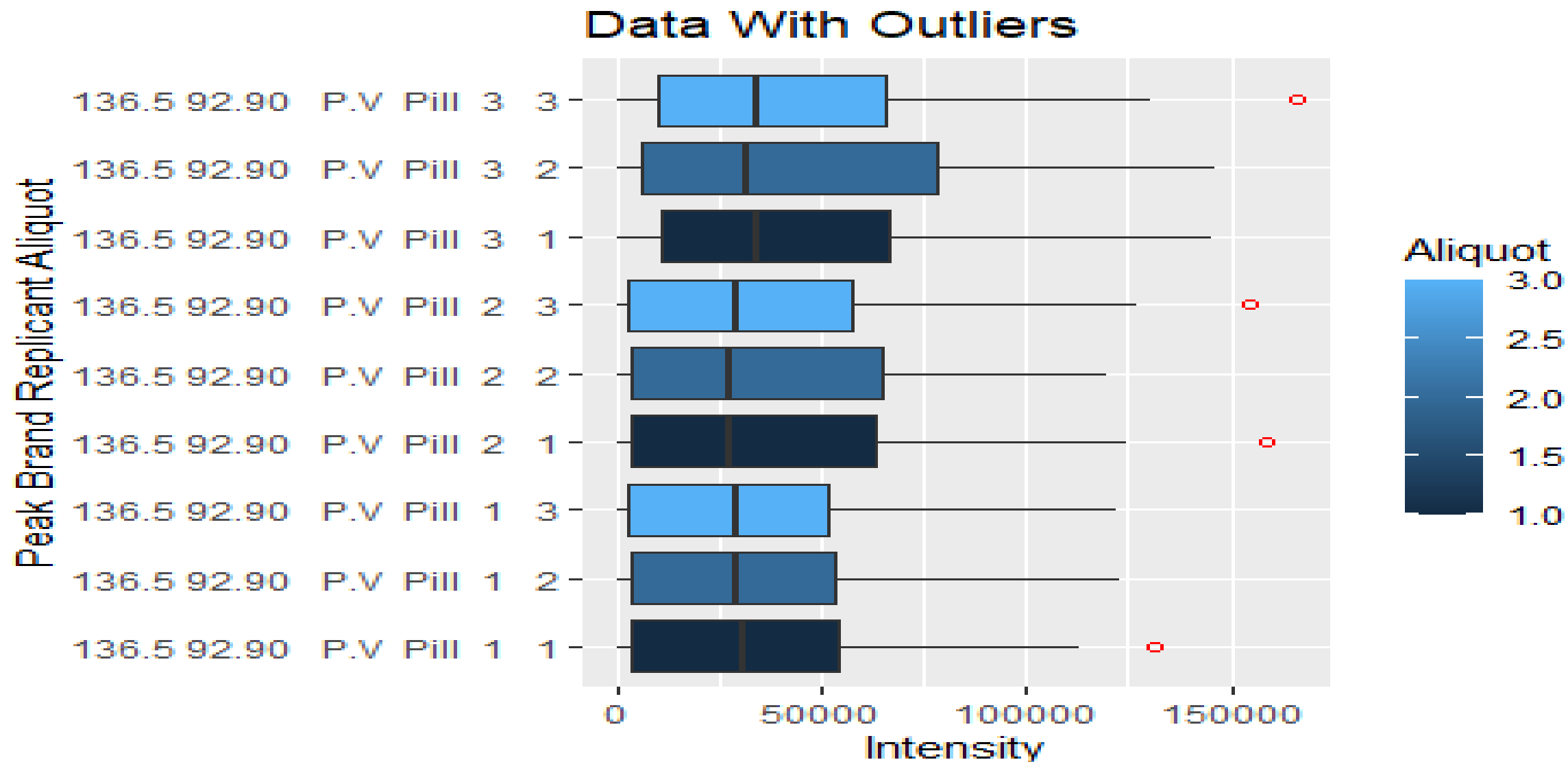
Exploratory Analysis



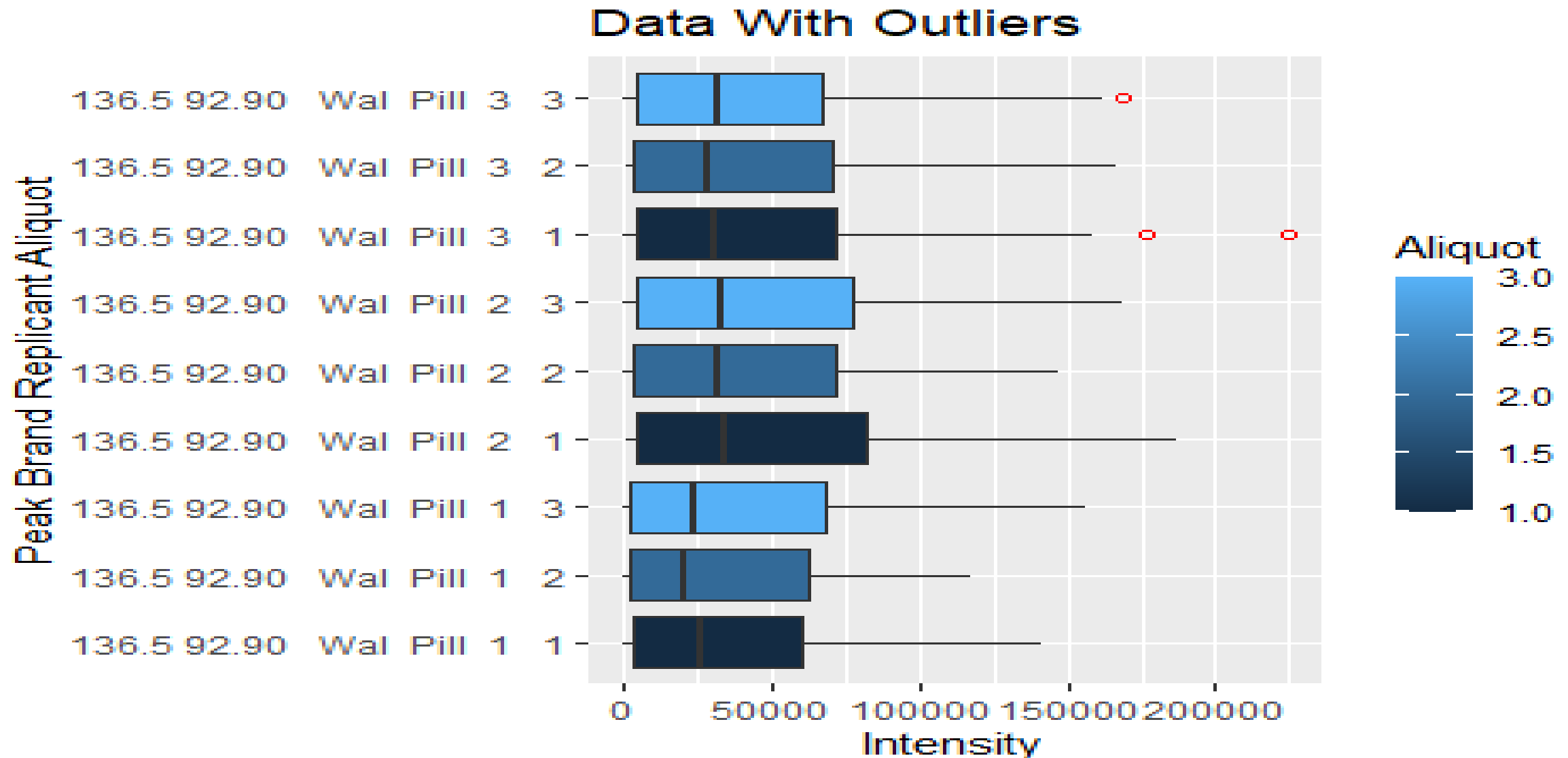
Exploratory Analysis



Exploratory Analysis



Exploratory Analysis



Analysis



One Way ANOVA and Pairwise comparisons of AUPs for each Brand

- Complete with an alpha of .5 to get a 95% confidence interval statistical significance comparison
- All 3 at once and pairwise comparisons using Student's t-distribution tests

Brand	AoV P Value	Pairwise T Test P Value
Brand - With Outliers	0.973	
Brand - w/o Outliers	0.729	
P.V. vs Bayer - With Outliers		0.85
Wal vs Bayer - With Outliers		0.98
Wal vs P.V. - With Outliers		0.83
P.V. vs Bayer - w/o Outliers		0.53
Wal vs Bayer - w/o Outliers		0.46
Wal vs P.V - w/o Outliers		0.91

Analysis

Ad-Hoc Pairwise comparisons

- Tukey-Kramer comparison which has an error correction that assists when comparing pairs within a group with sample sizes that aren't exactly the same.
- Bonferroni comparison which has an error correction that, similarly to the Tukey-Kramer test, also assists when comparing pairs within a group with sample sizes that aren't exactly the same.

Brand	Tukey_Kramer_P_Values	Bonferroni_P_Values
P.V. vs Bayer - With Outliers	0.489	0.818
Wal vs Bayer - With Outliers	0.984	0.887
Wal vs P.V. - With Outliers	0.389	0.118
P.V. vs Bayer - w/o Outliers	0.078	0.140
Wal vs Bayer - w/o Outliers	0.030	0.132
Wal vs P.V - w/o Outliers	0.924	0.624

Conclusions

Null Hypothesis that the Aspirin Pills Are the Same

- Failed to reject null hypothesis that the aspirin pills are the same
 - Initial ANOVA test revealed that at a 95% confidence interval, there is no difference between the brands with or without the outliers being removed
 - This result was confirmed when running pairwise t-tests between the 3 brands
- Ad-Hoc Analysis
 - When outliers are not removed and when comparing the individual brands between each other using either Tukey-Kramer or Bonferroni analyses, the null hypothesis is not rejected at a 95% confidence interval
 - When outliers are removed and the Tukey-Kramer analysis but not the Bonferroni analysis is used, the Walgreens and Bayers brand aspirin pills are found to be different at a 95% confidence interval, rejecting the null hypothesis
- Standard One-Way ANOVA is being prioritized and thus the null hypothesis fails to be rejected

Sources

- <https://www.vedantu.com/formula/anova-formula>
- <https://www.educba.com/t-test-formula/>
- <https://www.statology.org/tukey-vs-bonferroni-vs-scheffe/>
- <https://aaronshlegel.me/tukeys-test-post-hoc-analysis.html>
- <https://www.itl.nist.gov/div898/handbook/prc/section4/prc473.htm>
- <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3052391/>