

Statistical Analysis Report on Reaction Rate Study

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1 Executive Summary

- Exponential models were fit to the data and rates were estimated (see Table 1). Statistical comparison of rates between all pairs of conditions was performed and differences are reported in terms of statistical significance and magnitude of effect (see Tables 2 through 13).
- Ianite: Rates for Ianite loss differed significantly among buffers, with B showing the most and C the least (see Figure 1 (observed) or Figure 4 (fitted)).
- Zerbene: Although some comparisons among buffers were statistically significant, differences in rates were quite small (see Figure 2 (observed) or Figure 5 (fitted)).
- LL: There were significant differences in rates among buffers, with A showing the smallest rate at the higher temperatures (see Figure 3 (observed) or Figure 6 (fitted)).

2 Statistical Methods

For all responses, an exponential model was fit to each curve. The non-linear model was fit independently to each curve using the following equation:

$$Concentration = c_0 * e^{-kt}$$

In this model, c_0 is the initial concentration at time 0, k is the decay rate, and t is time in days. The models were also fit in their linearized form:

$$\ln(Concentration) = \ln(c_0) - kt$$

The linearized model was used for the purpose of statistical analysis and pairwise comparisons. Future work will include reanalysis using a non-linear model. Under the current approach, rates from the linearized model were compared to rates from independent exponential fits to confirm similarity. The linear model used in the statistical analysis estimated a separate rate for each buffer. One model was run for each response and temperature in the experiment. As long as the overall effect of buffer was found to be significant, all pairwise comparisons were made between buffer types.

Since low variability among replicate measurements led to most comparisons being statistically significant, even in cases where actual differences in rates were quite small, results were reported at various cutoff levels based on the magnitude of the rate difference.

3 Results

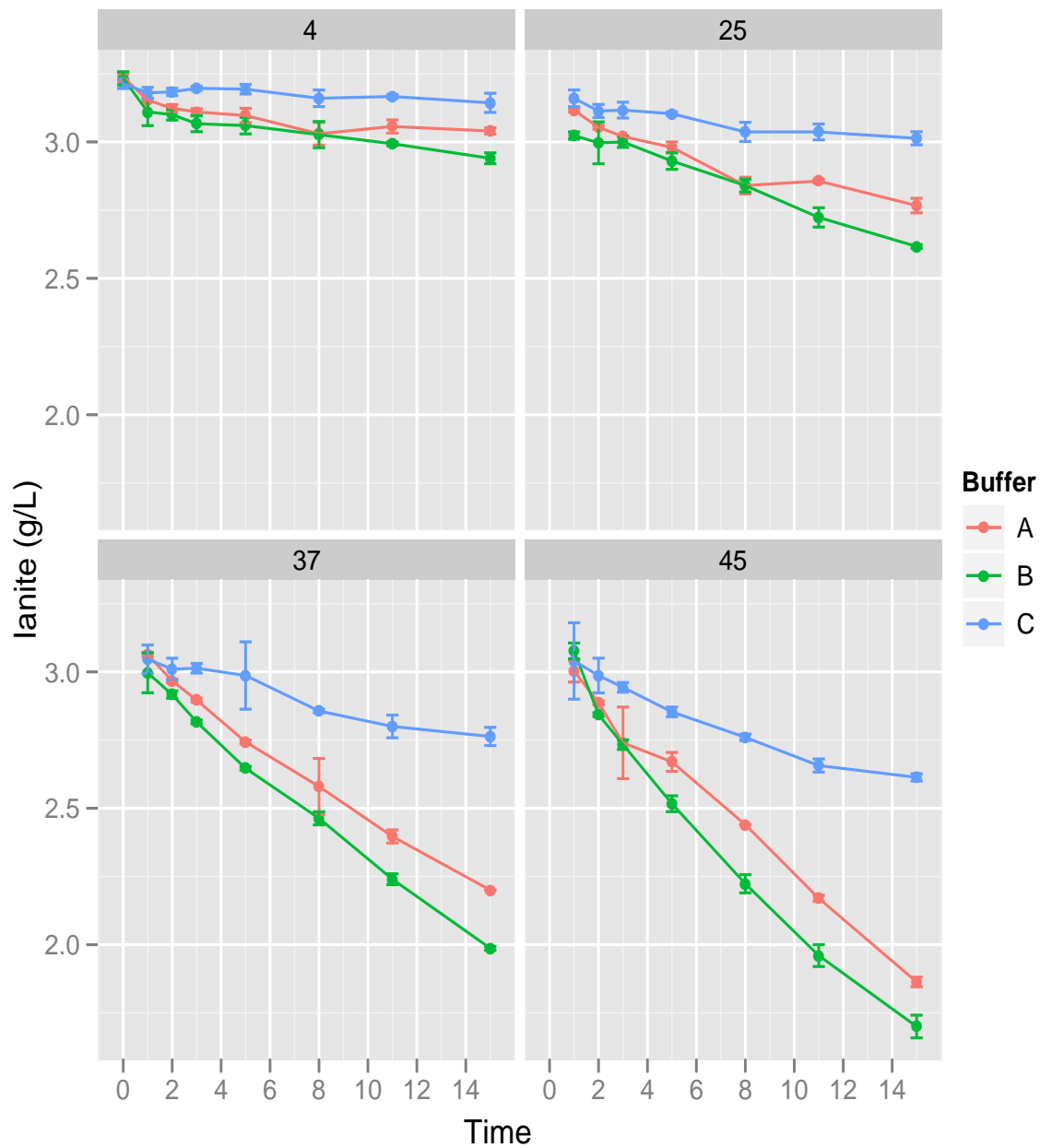


Figure 1: Ianite concentration change over time and temperature for each type. The mean \pm 2 standard errors of the observed data are displayed.

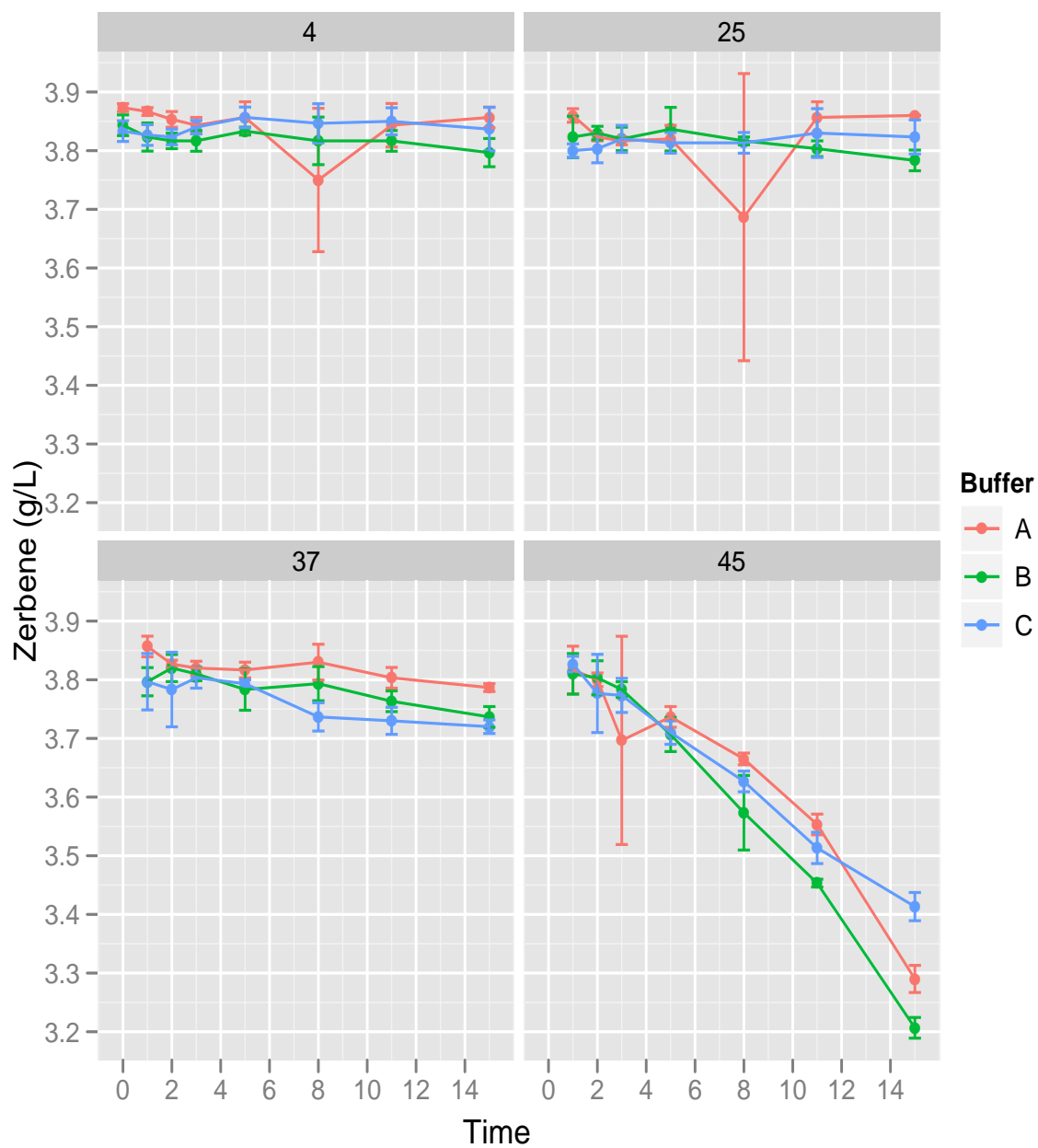


Figure 2: Zerbene concentration change over time and temperature for each type. The mean \pm 2 standard errors of the observed data are displayed.

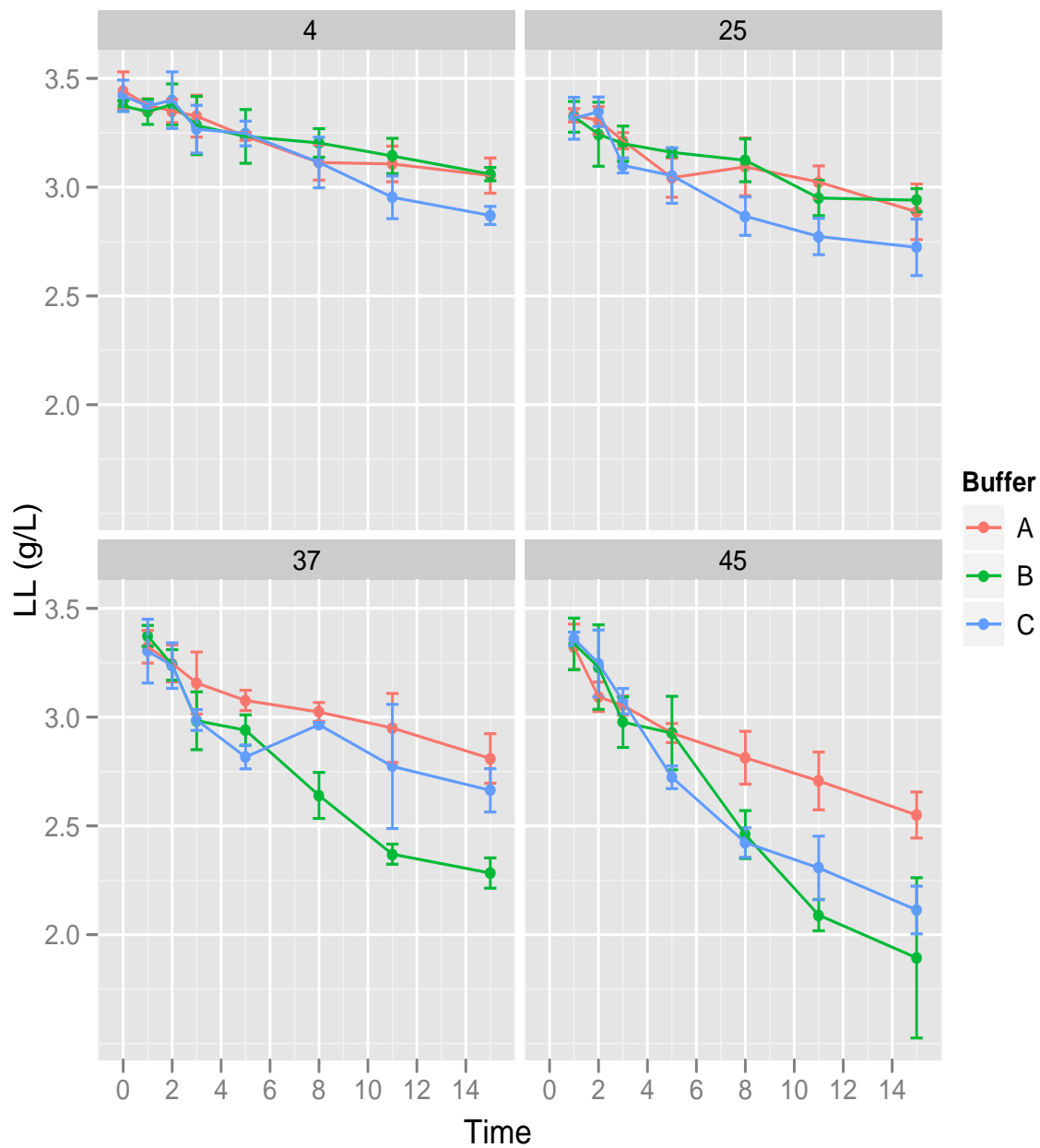


Figure 3: LL concentration change over time and temperature for each type. The mean \pm 2 standard errors of the observed data are displayed.

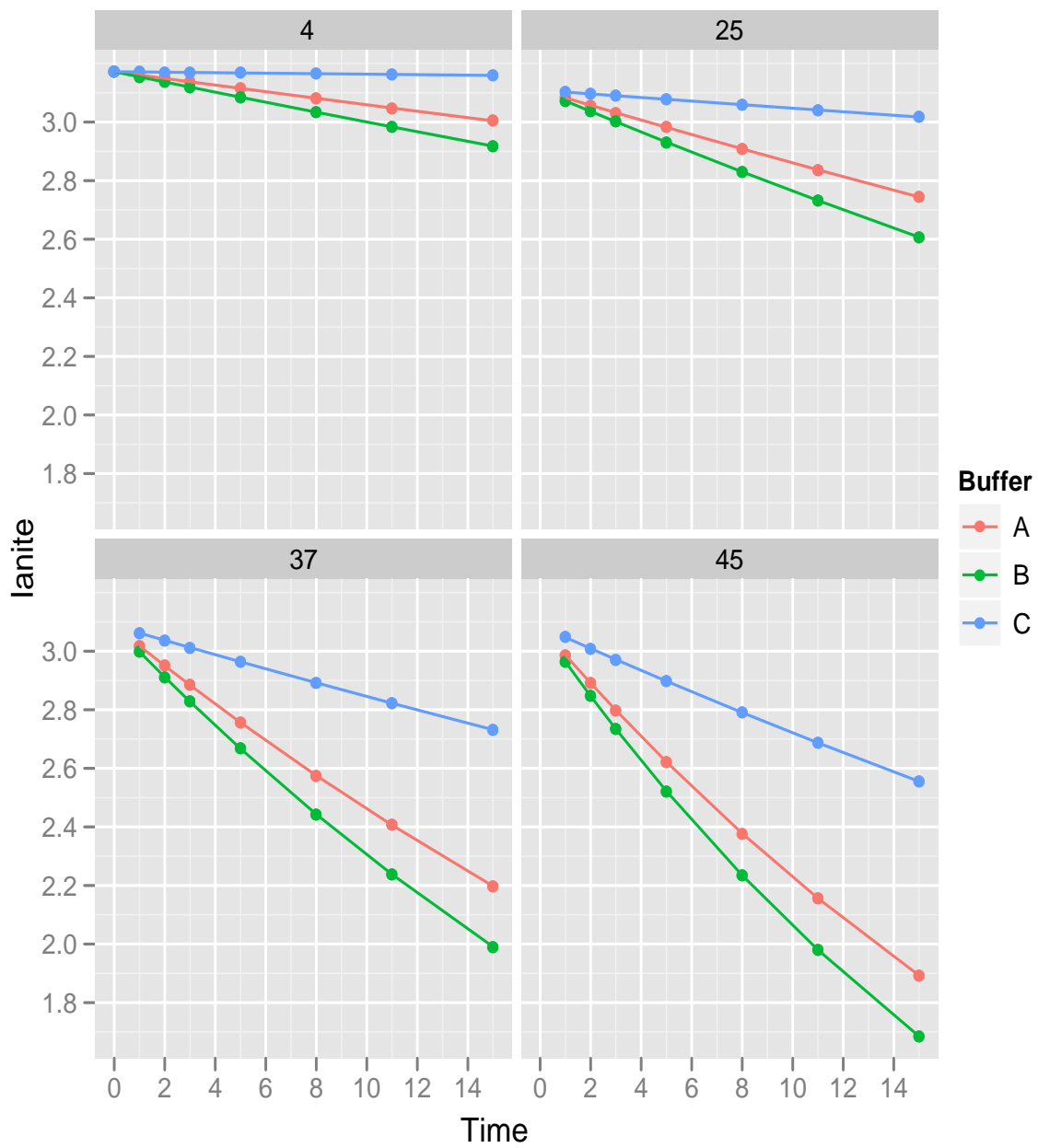


Figure 4: Ianite predicted concentrations based on the fitted model.

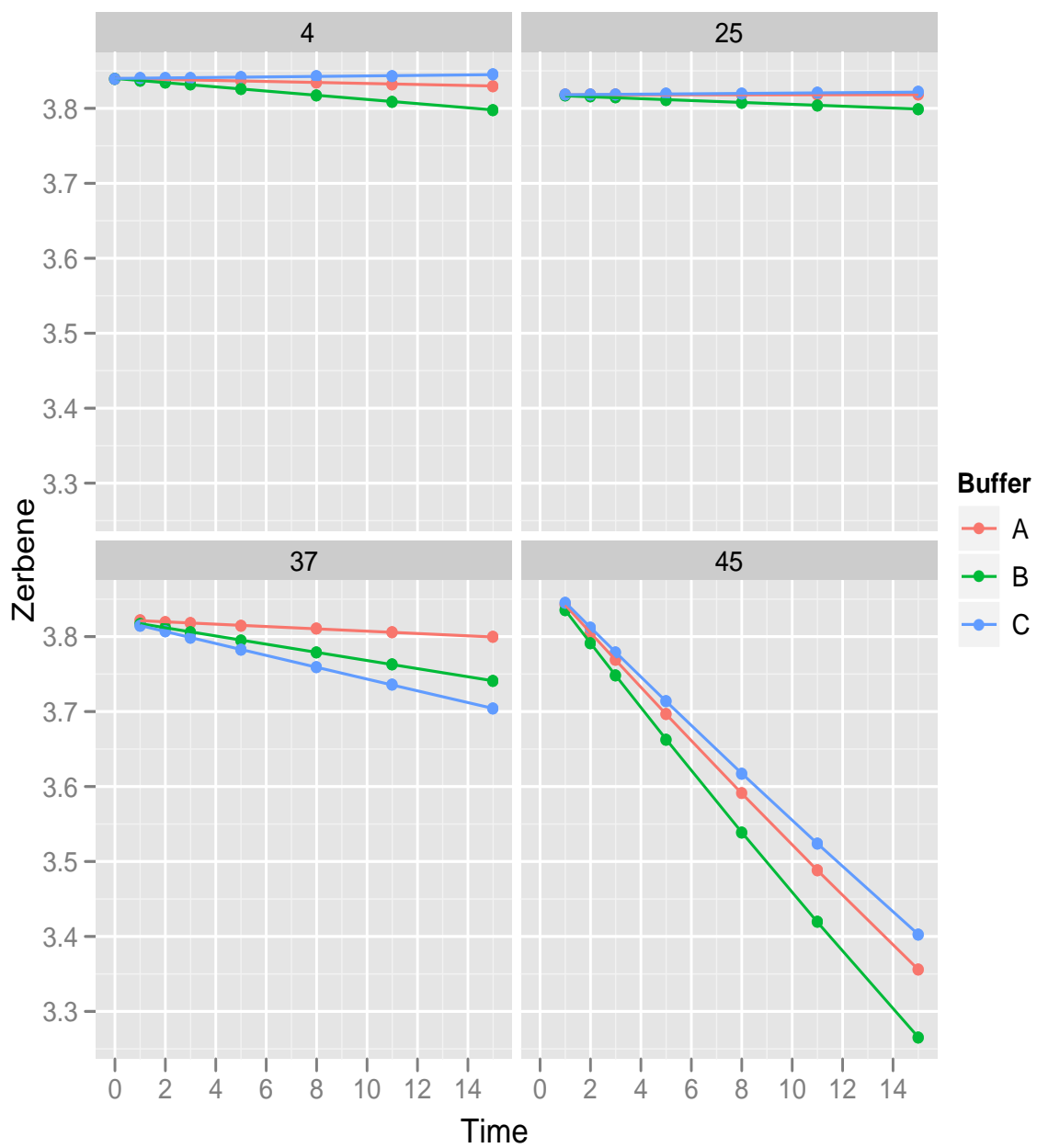


Figure 5: Zerbene predicted concentrations based on the fitted model.

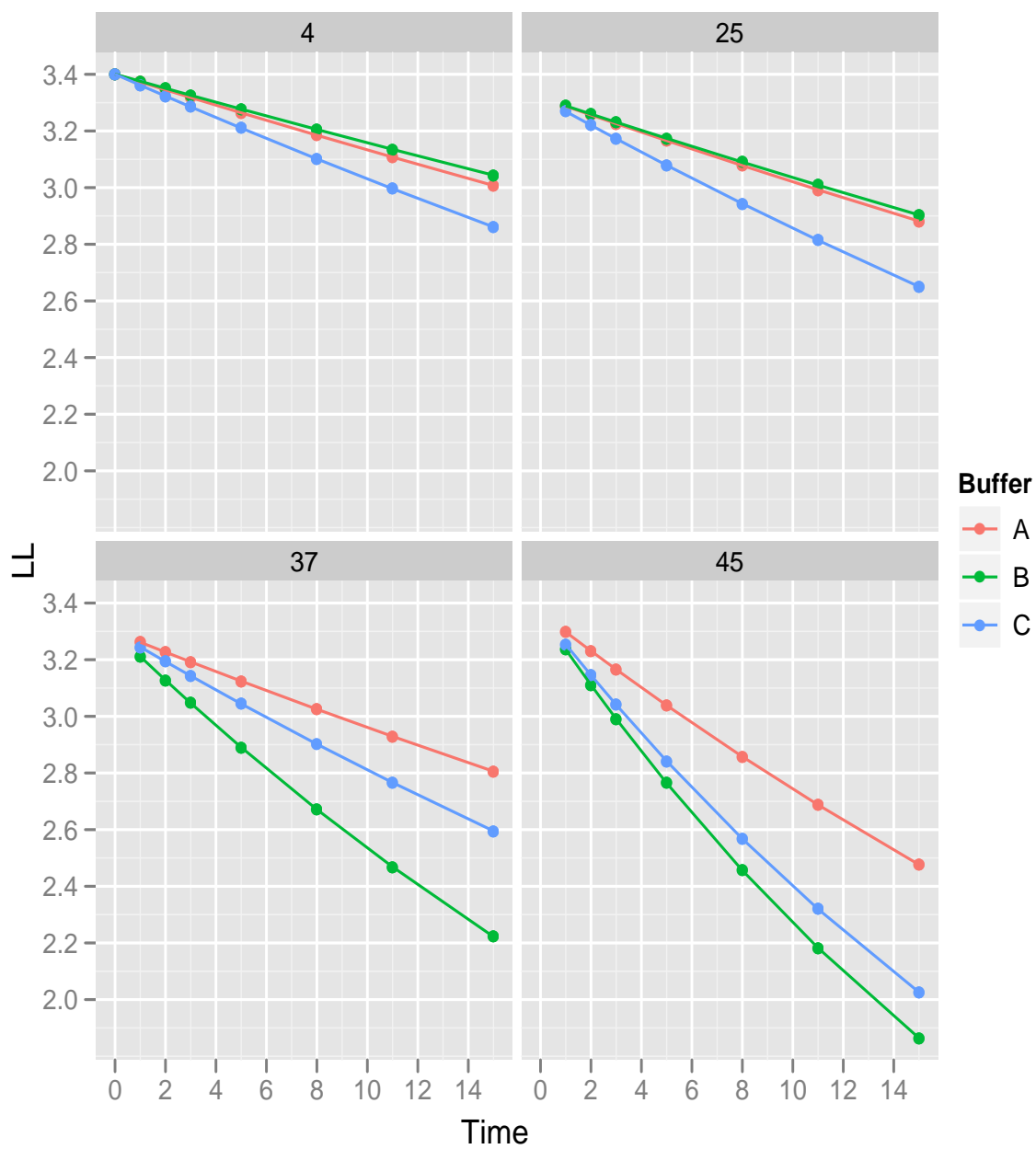


Figure 6: LL predicted concentrations based on the fitted model.

Response	Temperature	A	B	C
Ianite	4	3.60	5.60	0.26
Ianite	25	8.30	12.00	2.00
Ianite	37	23.00	29.00	8.20
Ianite	45	33.00	40.00	13.00
Zerbene	4	0.18	0.73	-0.09
Zerbene	25	-0.00	0.33	-0.06
Zerbene	37	0.41	1.40	2.10
Zerbene	45	9.70	11.00	8.70
LL	4	8.20	7.40	12.00
LL	25	9.40	8.90	15.00
LL	37	11.00	26.00	16.00
LL	45	20.00	39.00	34.00

Table 1: Estimated rates from exponential model (10^{-3}).

	A	B	C
A	-	>0.0	>0.0
B	>0.0	-	>0.0
C	>0.0	>0.0	-

Table 2: Statistical results of comparisons among all buffers for Ianite at 4 degrees. NS indicates non-significant comparisons. >x.x indicates a significant difference for the comparison ($p < .05$), with the difference in rates being significantly greater than x.x. >0.0 indicates a statistically significant difference in rates where the difference is less than 0.01.

	A	B	C
A	-	>0.0	>0.0
B	>0.0	-	>0.0
C	>0.0	>0.0	-

Table 3: Statistical results of comparisons among all buffers for Ianite at 25 degrees.

	A	B	C
A	-	>0.0	>0.01
B	>0.0	-	>0.02
C	>0.01	>0.02	-

Table 4: Statistical results of comparisons among all buffers for Ianite at 37 degrees.

	A	B	C
A	-	>0.0	>0.01
B	>0.0	-	>0.02
C	>0.01	>0.02	-

Table 5: Statistical results of comparisons among all buffers for Ianite at 45 degrees.

	A	B	C
A	-	NS	NS
B	NS	-	NS
C	NS	NS	-

Table 6: Statistical results of comparisons among all buffers for Zerbene at 4 degrees. NS indicates non-significant comparisons. >x.x indicates a significant difference for the comparison ($p < .05$), with the difference in rates being significantly greater than x.x. >0.0 indicates a statistically significant difference in rates where the difference is less than 0.01.

	A	B	C
A	-	NS	NS
B	NS	-	NS
C	NS	NS	-

Table 7: Statistical results of comparisons among all buffers for Zerbene at 25 degrees.

	A	B	C
A	-	>0.0	>0.0
B	>0.0	-	>0.0
C	>0.0	>0.0	-

Table 8: Statistical results of comparisons among all buffers for Zerbene at 37 degrees.

	A	B	C
A	-	>0.0	NS
B	>0.0	-	>0.0
C	NS	>0.0	-

Table 9: Statistical results of comparisons among all buffers for Zerbene at 45 degrees.

	A	B	C
A	-	NS	>0.0
B	NS	-	>0.0
C	>0.0	>0.0	-

Table 10: Statistical results of comparisons among all buffers for LL at 4 degrees. NS indicates non-significant comparisons. >x.x indicates a significant difference for the comparison ($p < .05$), with the difference in rates being significantly greater than x.x. >0.0 indicates a statistically significant difference in rates where the difference is less than 0.01.

	A	B	C
A	-	NS	>0.0
B	NS	-	>0.0
C	>0.0	>0.0	-

Table 11: Statistical results of comparisons among all buffers for LL at 25 degrees.

	A	B	C
A	-	>0.01	>0.0
B	>0.01	-	>0.0
C	>0.0	>0.0	-

Table 12: Statistical results of comparisons among all buffers for LL at 37 degrees.

	A	B	C
A	-	>0.01	>0.0
B	>0.01	-	>0.0
C	>0.0	>0.0	-

Table 13: Statistical results of comparisons among all buffers for LL at 45 degrees.