

CH Activation - Model Testing

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formula	McFadden R2
class ~ diff_9_13 + Total_1 + Dist(9, 13) + Aniso.Polar	0.790
class ~ B1_2 + B1_3 + diff_10_Metalla + Dist(3, 9)	0.778
class ~ diff_3_4 + diff_10_Metalla + Dist(9, 13) + Dist(3, 9)	0.764
class ~ diff_3_9 + diff_9_Metalla + dip_z_1 + Dist(3, 9)	0.759
class ~ NPA_13 + Total_1 + Dist(9, 13) + Aniso.Polar	0.753
class ~ NPA_Metallic + diff_3_4 + Dist(9, 13) + Dist(3, 9)	0.753
class ~ B1_2 + diff_9_13 + diff_10_Metalla + Dist(9, 13)	0.750
class ~ B1_1 + NPA_13 + diff_10_Metalla + Dist(9, 13)	0.749
class ~ diff_3_4 + diff_10_Metalla + dip_y_1 + Dist(3, 9)	0.749
class ~ B1_2 + NPA_13 + diff_10_Metalla + Dist(9, 13)	0.748

Section Results Summary

	Training Accuracy	Test Accuracy
1. 1st Place	87.50	88.9
2. 2nd Place	87.50	88.9
3. 3rd Place	91.67	100.0
4. 4th Place	89.58	77.8
5. 5th Place	81.25	88.9
6. 6th Place	89.58	100.0
7. 7th Place	87.50	100.0
8. 8th Place	87.50	33.3
9. 9th Place	85.42	100.0

	Training Accuracy	Test Accuracy
10. 10th Place	89.58	100.0

1st Place

Table:

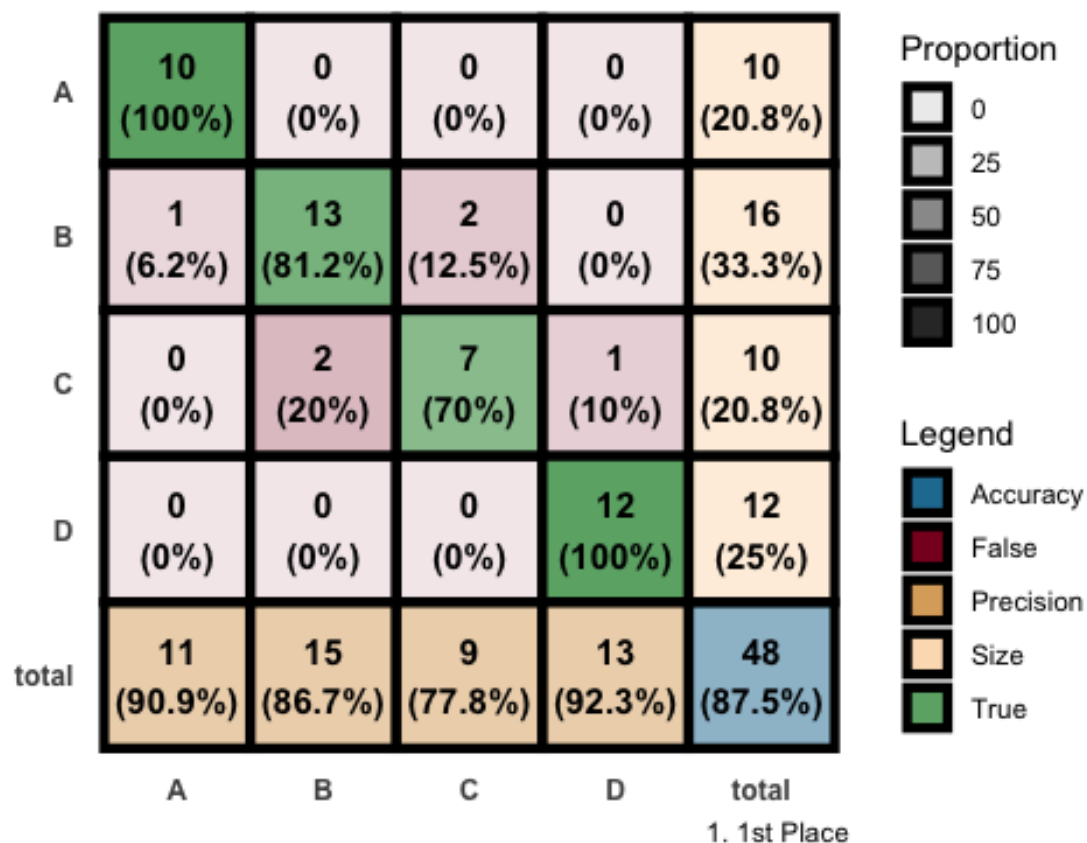
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
87.5%	0.79

Model Coefficients

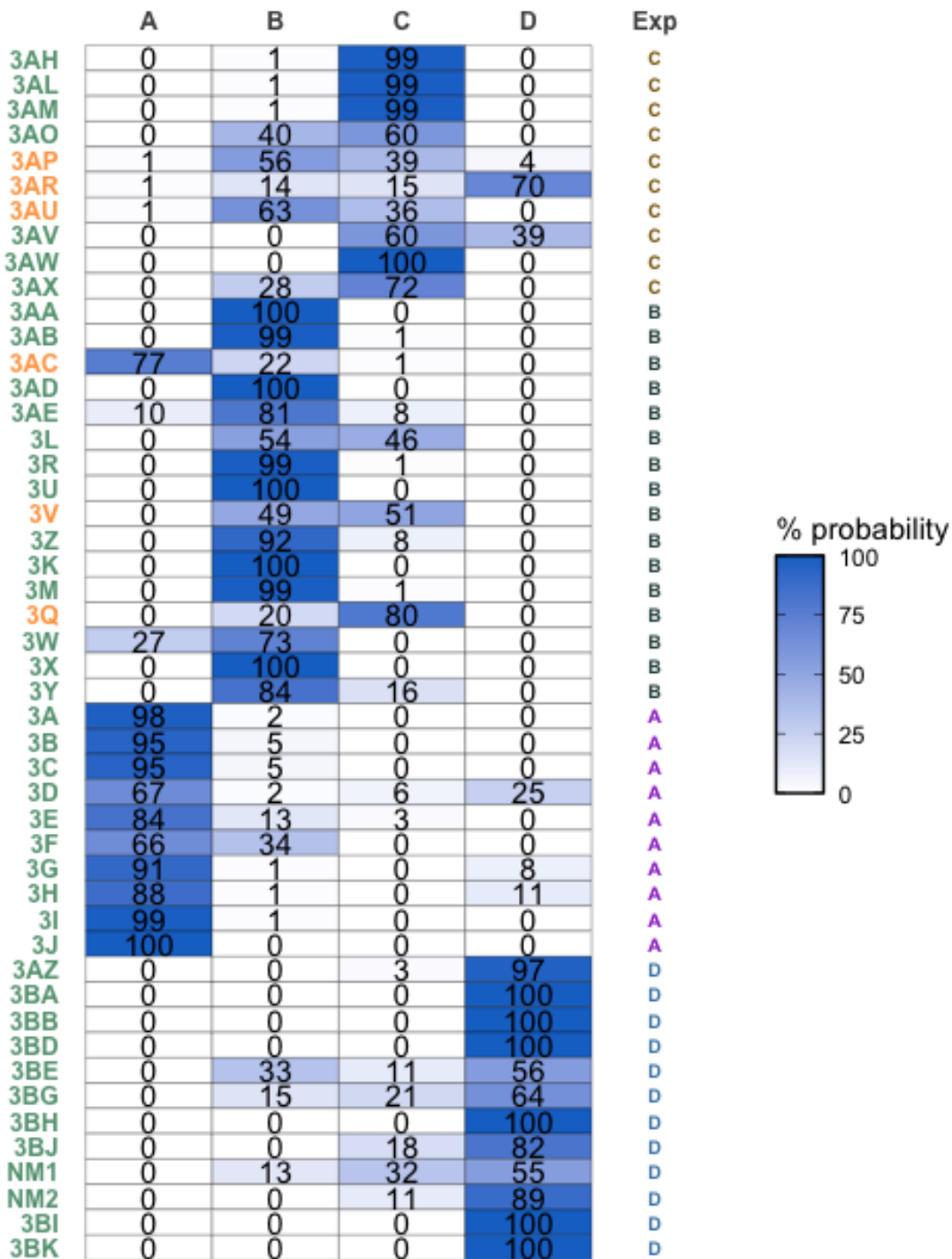
	(Intercept)	diff_9_13	Total_1	Dist(9, 13)	Aniso.Polar
2	398.7937	-35.68063	-0.2415319	-289.9721	0.0618394
3	372.5344	-37.07579	1.8363627	-269.2959	-0.0146075
4	-173.6428	-10.16339	6.6560566	170.4070	-0.6655851

Training Set Confusion Matrix



Training Set

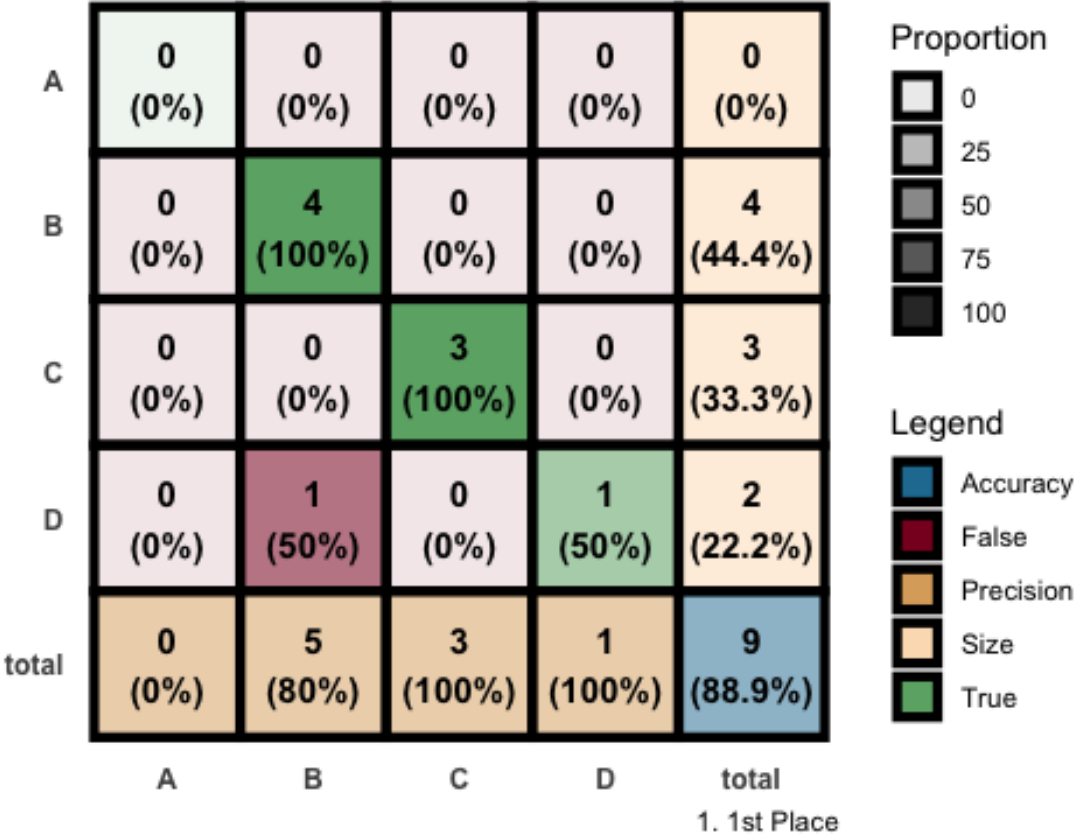
Probability Heatmap



1. 1st Place

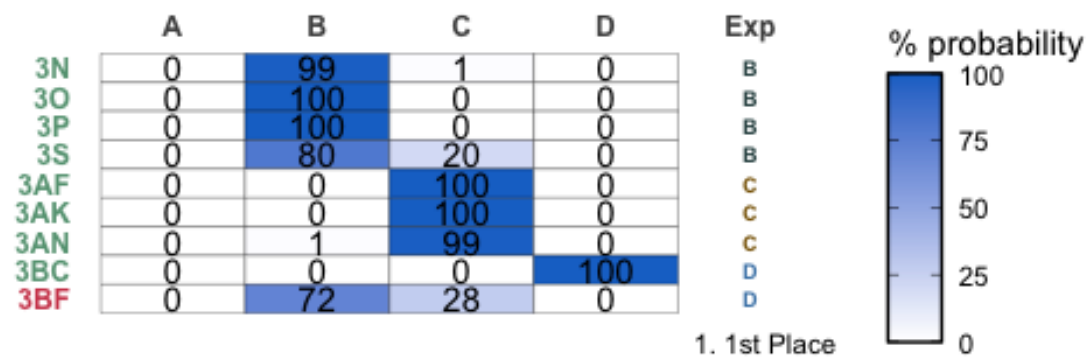
Test Set

Confusion Matrix



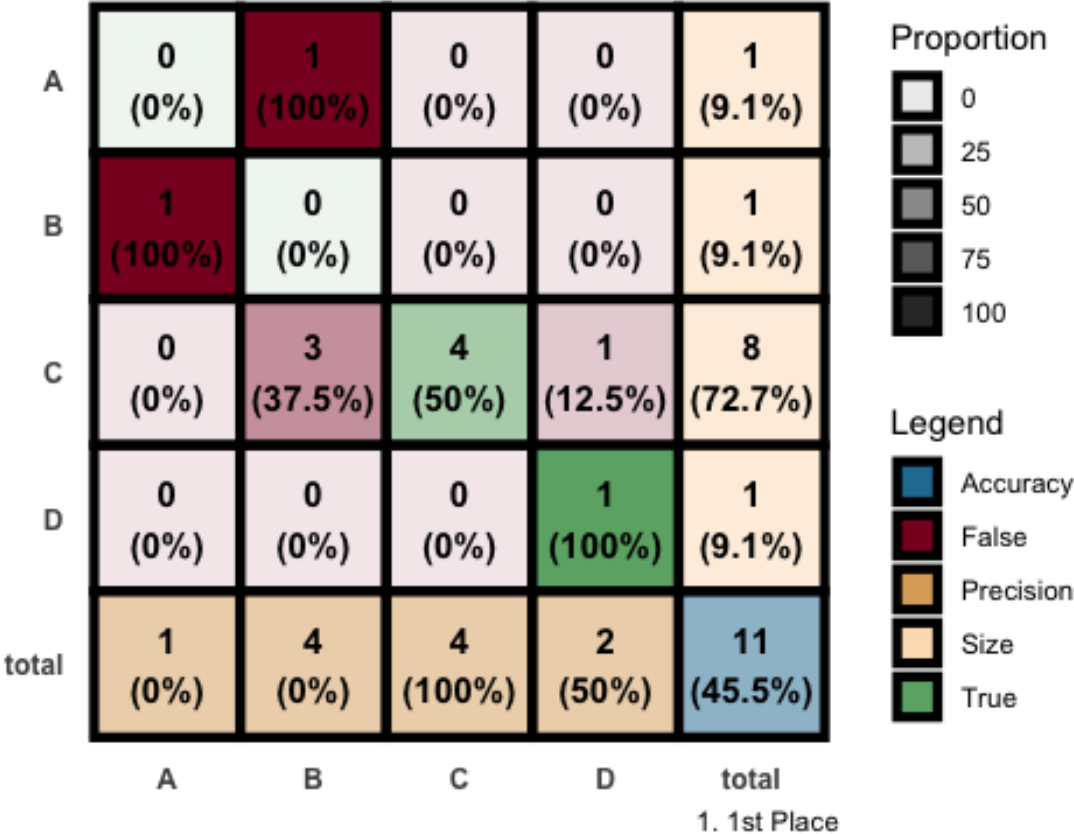
Test Set

Probability Heatmap



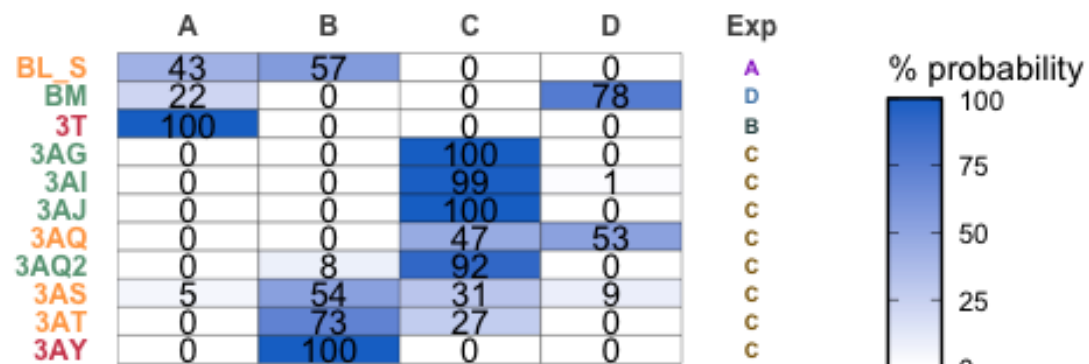
External Validation

Confusion Matrix



External Validation

Probability Heatmap



1. 1st Place

2nd Place

Table:

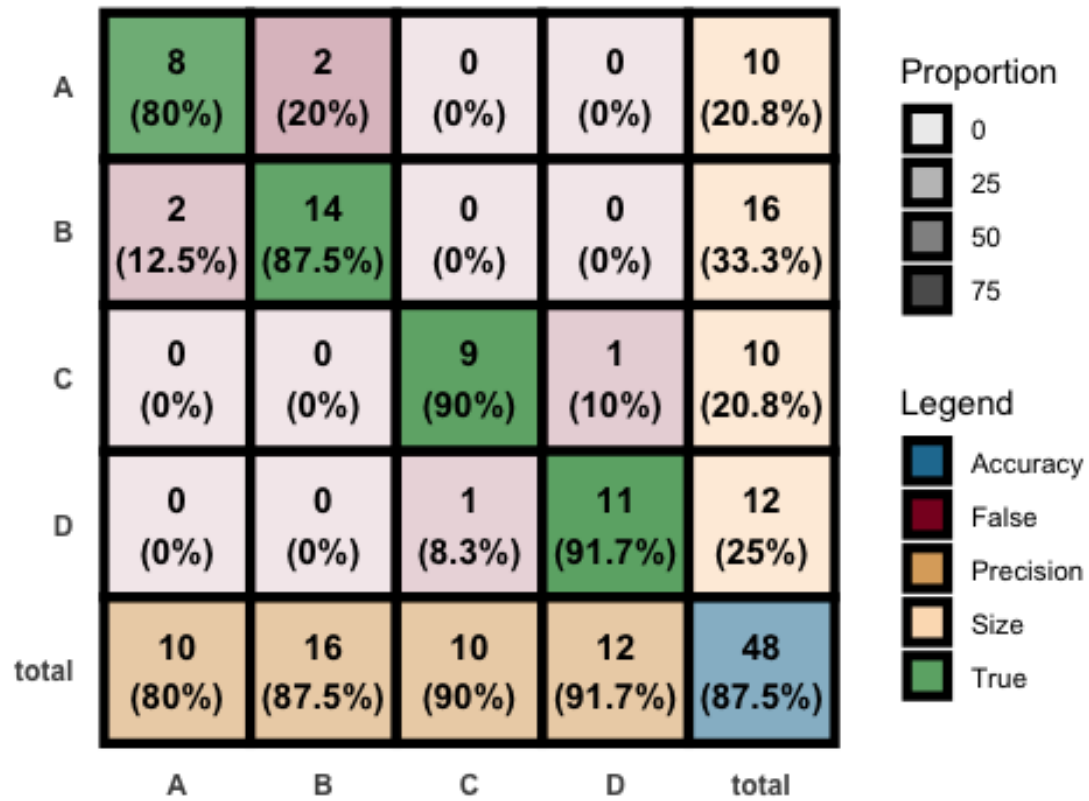
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
87.5%	0.778

Model Coefficients

	(Intercept)	B1_2	B1_3	diff_10_Metalla	Dist(3, 9)
2	211.8746	13.76068	-8.112532	62.63579	-179.38362
3	-221.8871	75.37330	-13.381946	440.53071	-152.67665
4	-314.3840	64.08609	27.417079	396.53425	-99.85631

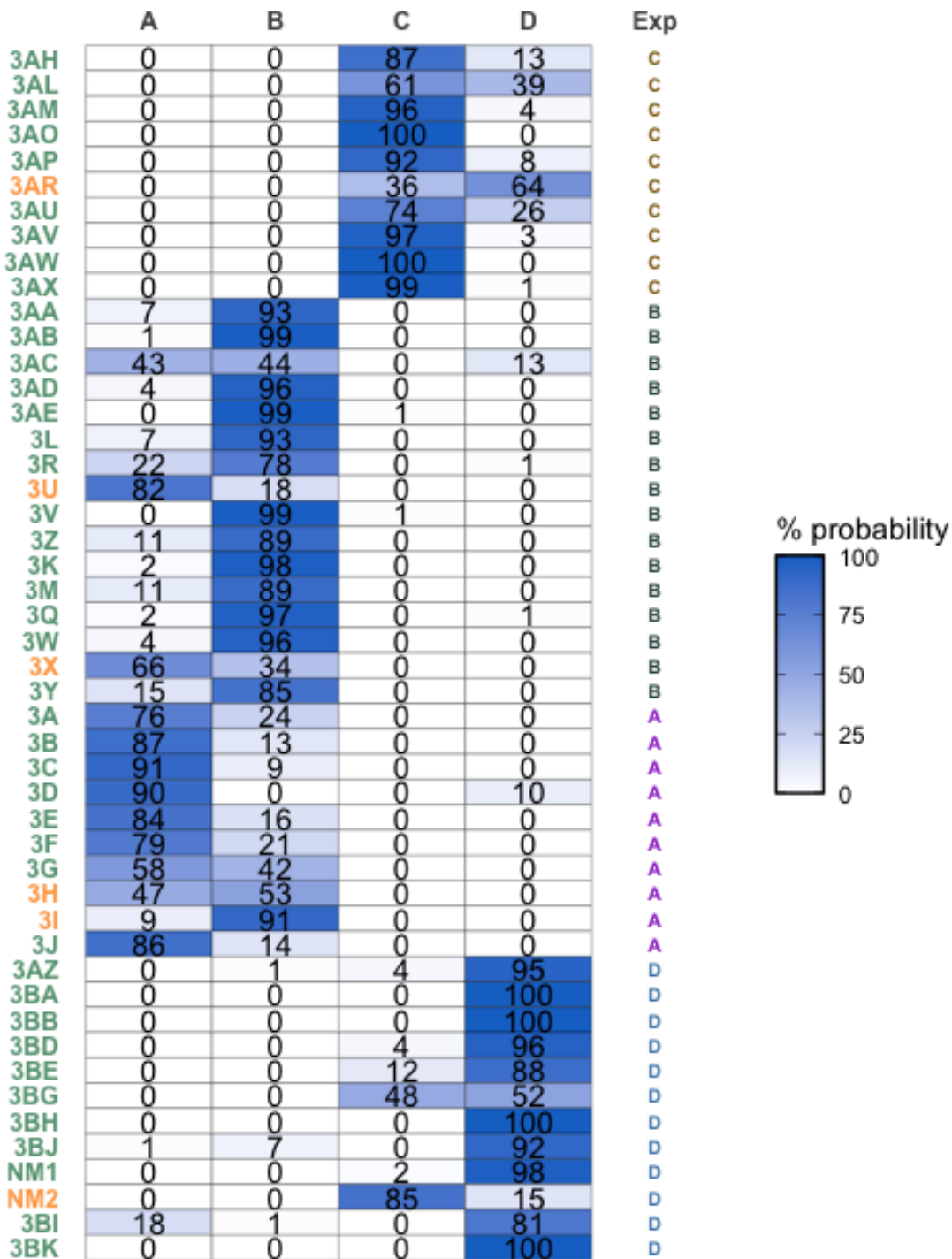
Training Set Confusion Matrix



2. 2nd Place

Training Set

Probability Heatmap



2. 2nd Place

Test Set

Confusion Matrix

A	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
B	0 (0%)	3 (75%)	0 (0%)	1 (25%)	4 (44.4%)
C	0 (0%)	0 (0%)	3 (100%)	0 (0%)	3 (33.3%)
D	0 (0%)	0 (0%)	0 (0%)	2 (100%)	2 (22.2%)
total	0 (0%)	3 (100%)	3 (100%)	3 (66.7%)	9 (88.9%)
	A	B	C	D	total

Proportion



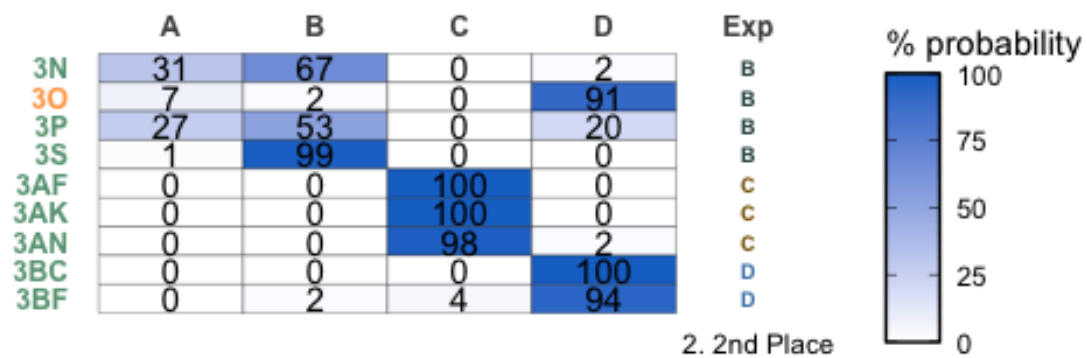
Legend



2. 2nd Place

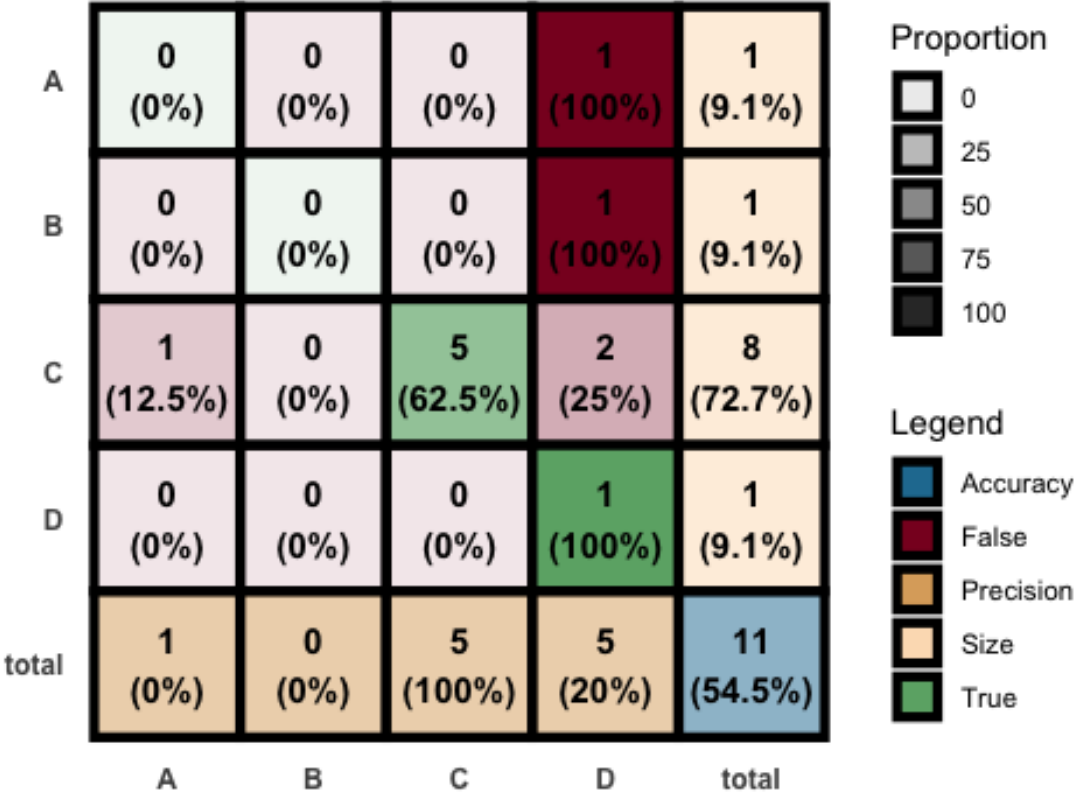
Test Set

Probability Heatmap



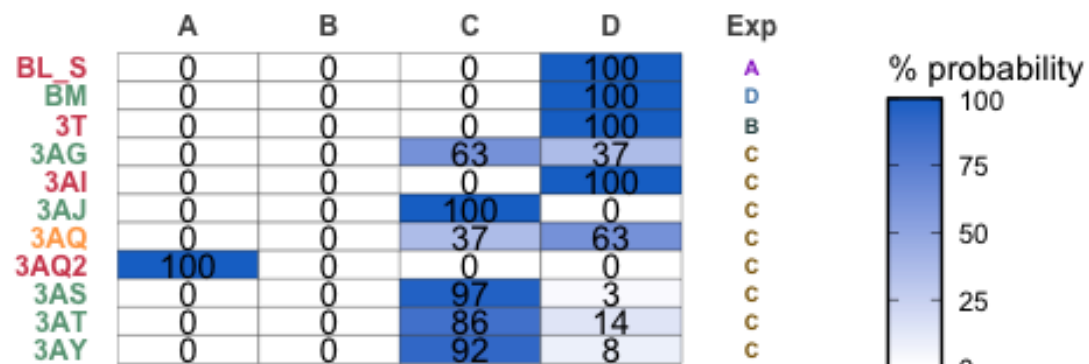
External Validation

Confusion Matrix



External Validation

Probability Heatmap



2. 2nd Place

3rd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

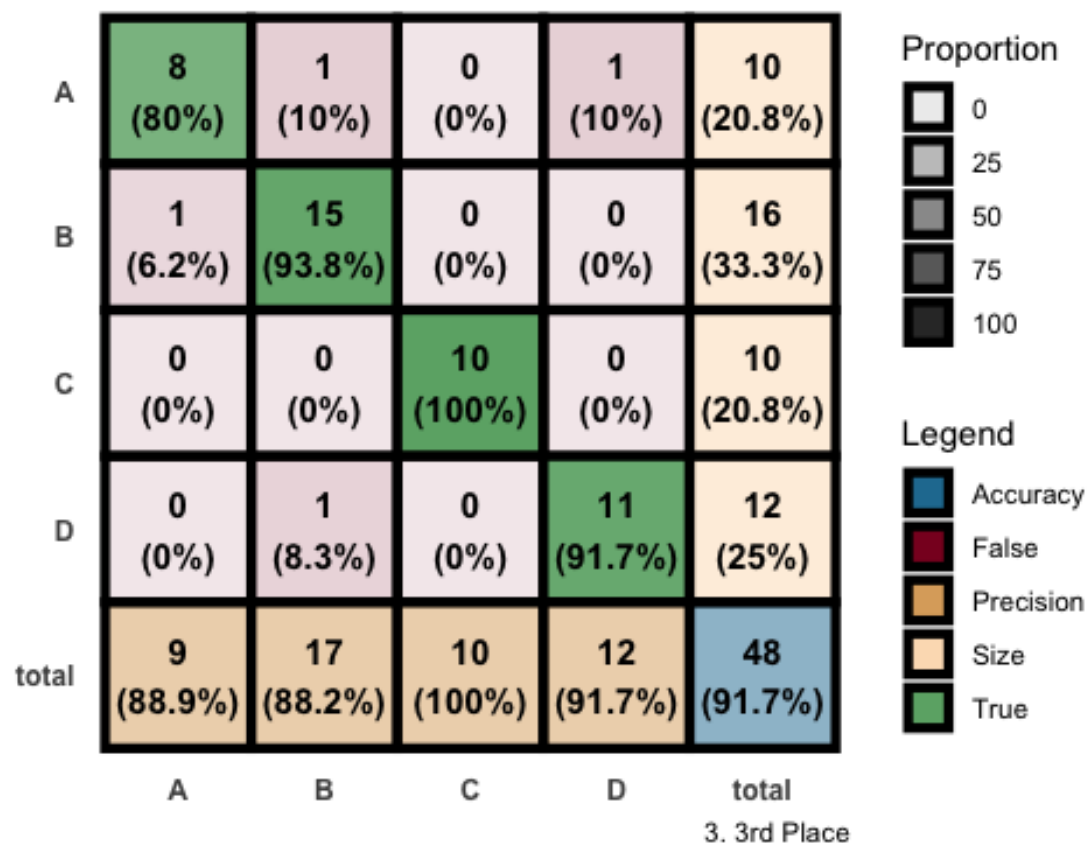
Accuracy	McFadden_R2
91.67%	0.764

Model Coefficients

	(Intercept)	diff_3_4	diff_10_Metalla	Dist(9, 13)	Dist(3, 9)
2	257.12219	-14.19944	7.125065	-28.49781	-151.9040
3	42.10109	292.02301	420.902411	-521.37798	157.0550
4	-255.57669	68.12549	19.771643	-49.91967	202.5617

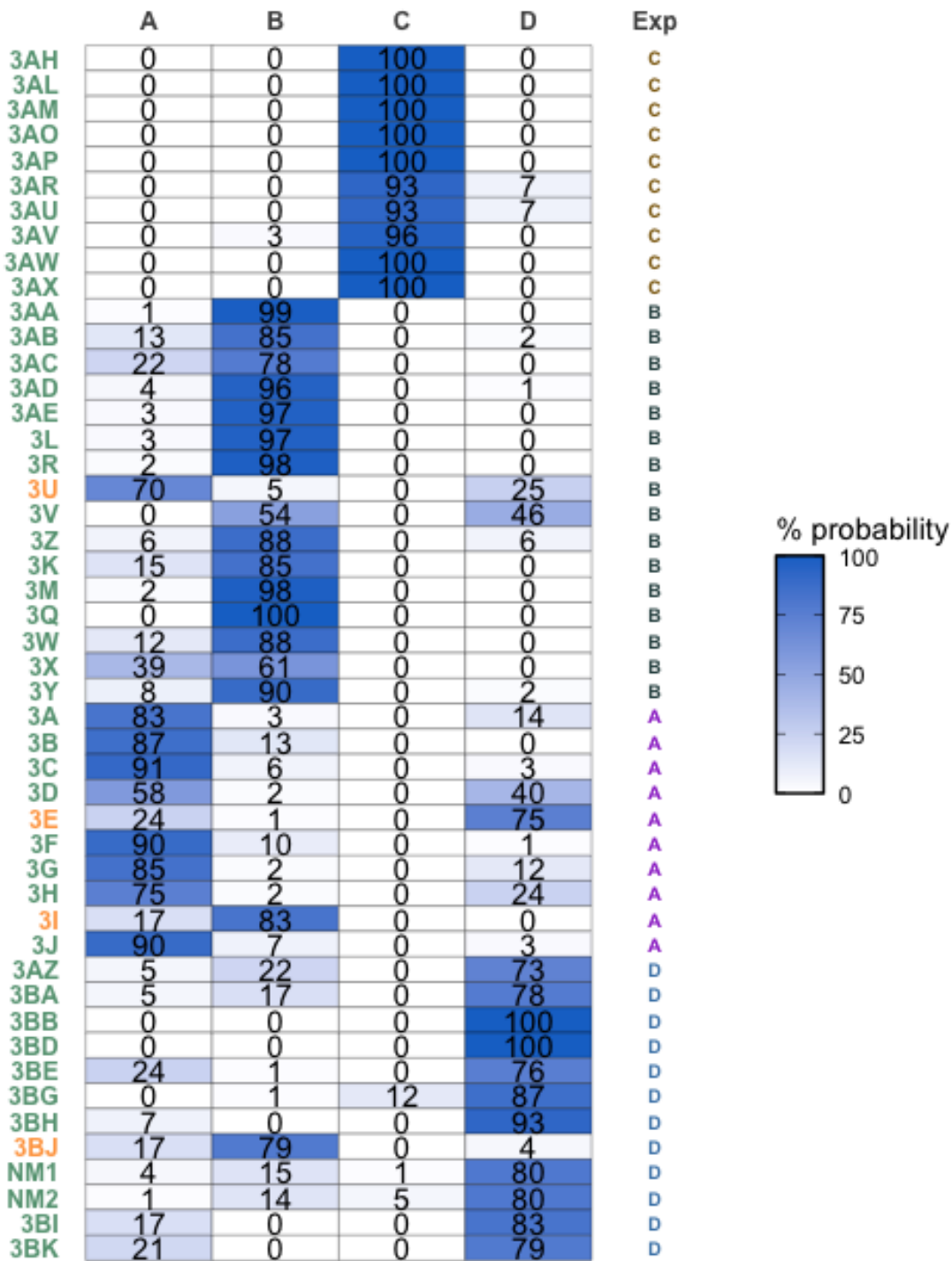
Training Set

Confusion Matrix



Training Set

Probability Heatmap



3. 3rd Place

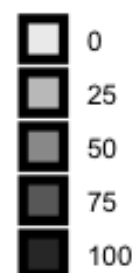
Test Set

Confusion Matrix

A	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
B	0 (0%)	4 (100%)	0 (0%)	0 (0%)	4 (44.4%)
C	0 (0%)	0 (0%)	3 (100%)	0 (0%)	3 (33.3%)
D	0 (0%)	0 (0%)	0 (0%)	2 (100%)	2 (22.2%)
total	0 (0%)	4 (100%)	3 (100%)	2 (100%)	9 (100%)
	A	B	C	D	total

3. 3rd Place

Proportion

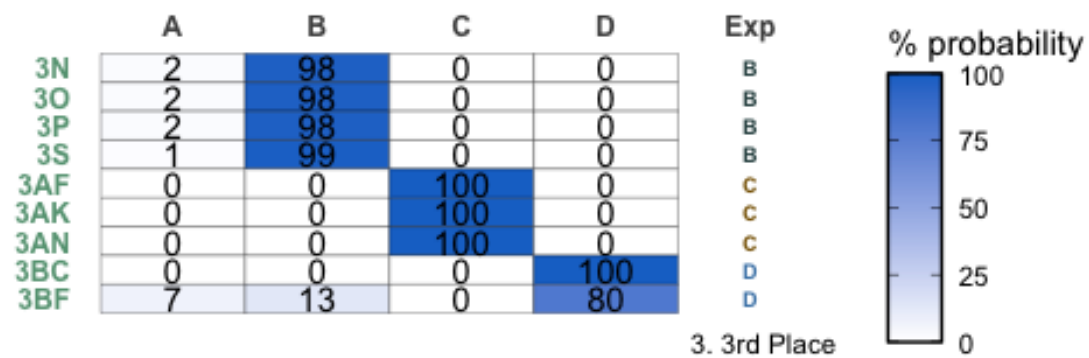


Legend



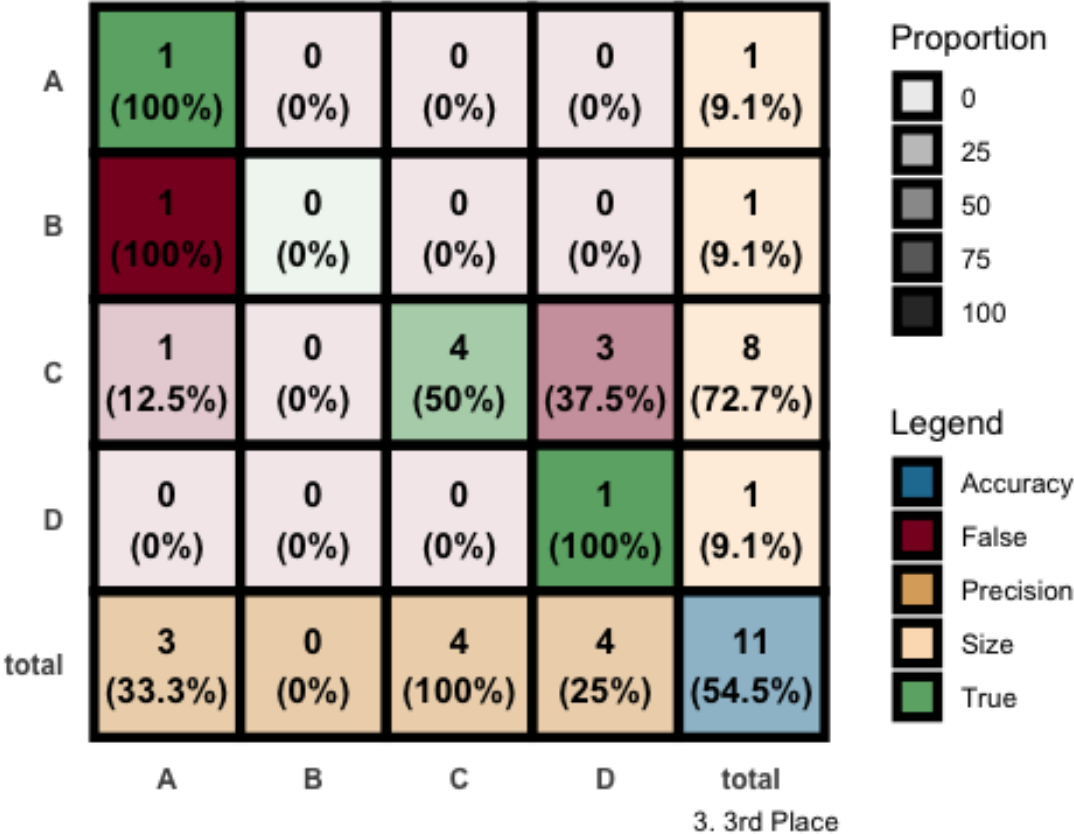
Test Set

Probability Heatmap



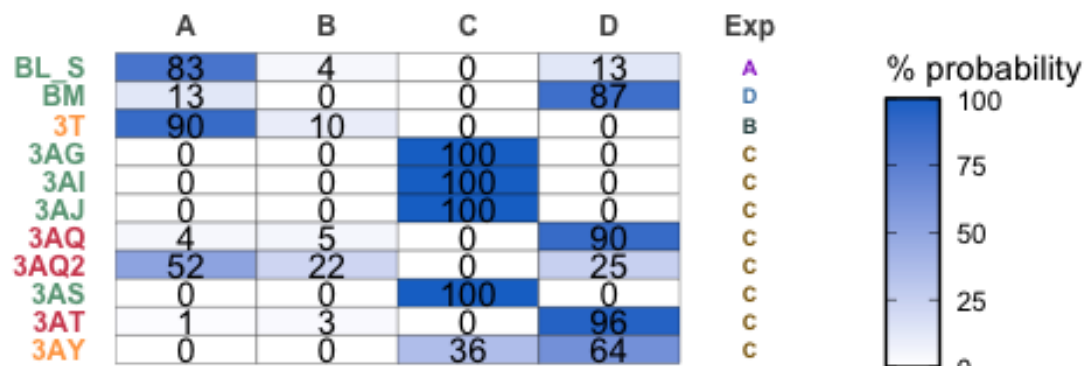
External Validation

Confusion Matrix



External Validation

Probability Heatmap



3. 3rd Place

4th Place

Table:

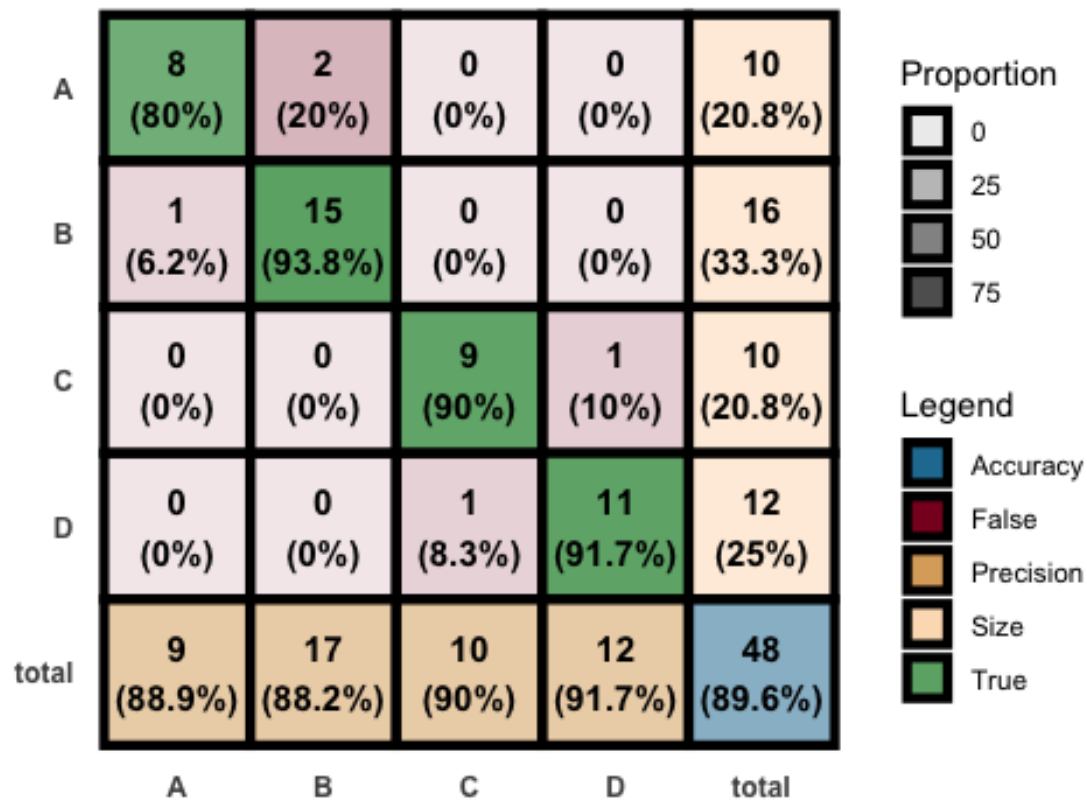
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
89.58%	0.759

Model Coefficients

	(Intercept)	diff_3_9	diff_9_Metalla	dip_z_1	Dist(3, 9)
2	212.5936	18.75626	-13.04726	0.7174497	-141.9147
3	-402.4659	-180.35054	211.81418	-5.1434922	194.7227
4	-732.0543	-124.65340	124.99069	-6.6957254	456.2272

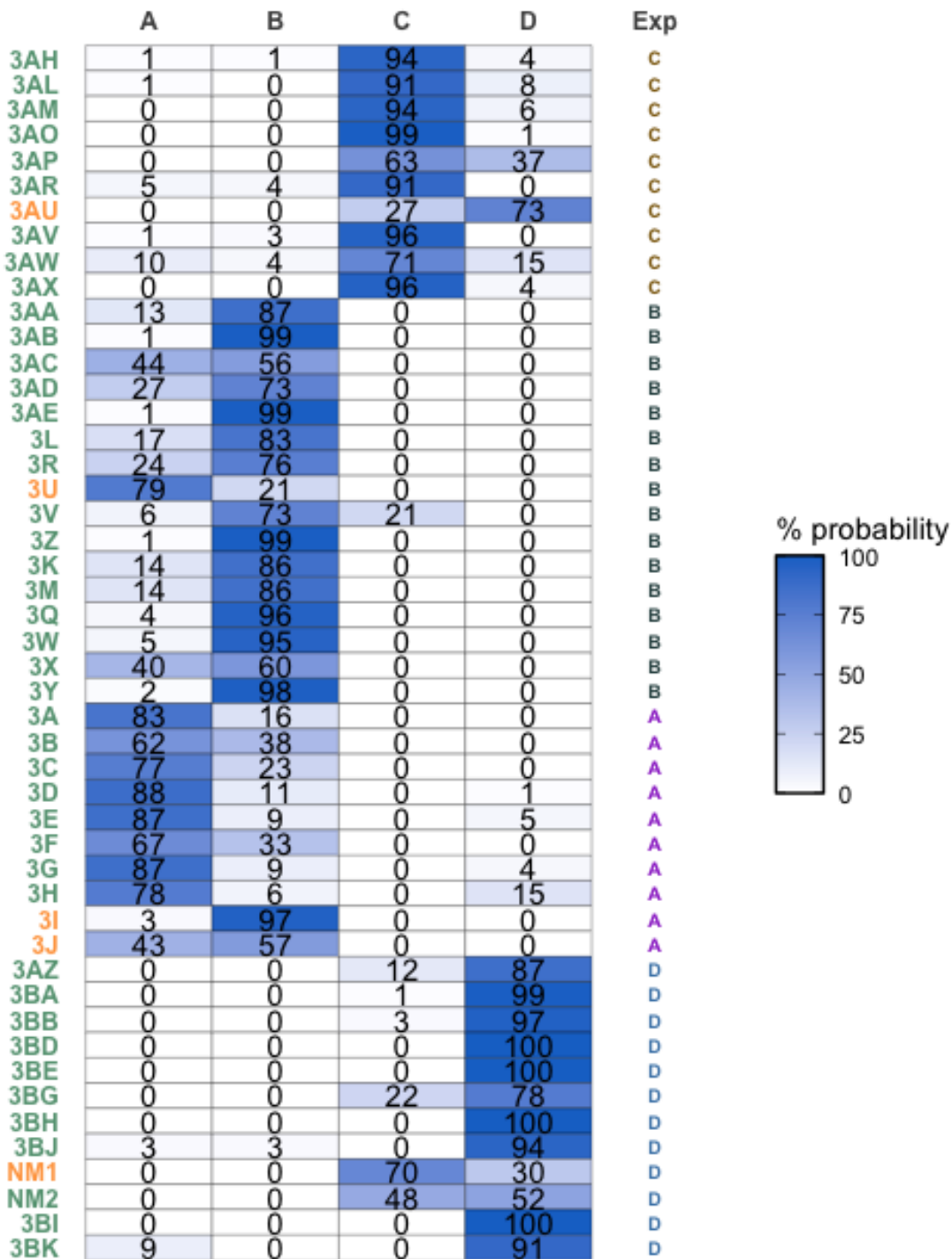
Training Set Confusion Matrix



4. 4th Place

Training Set

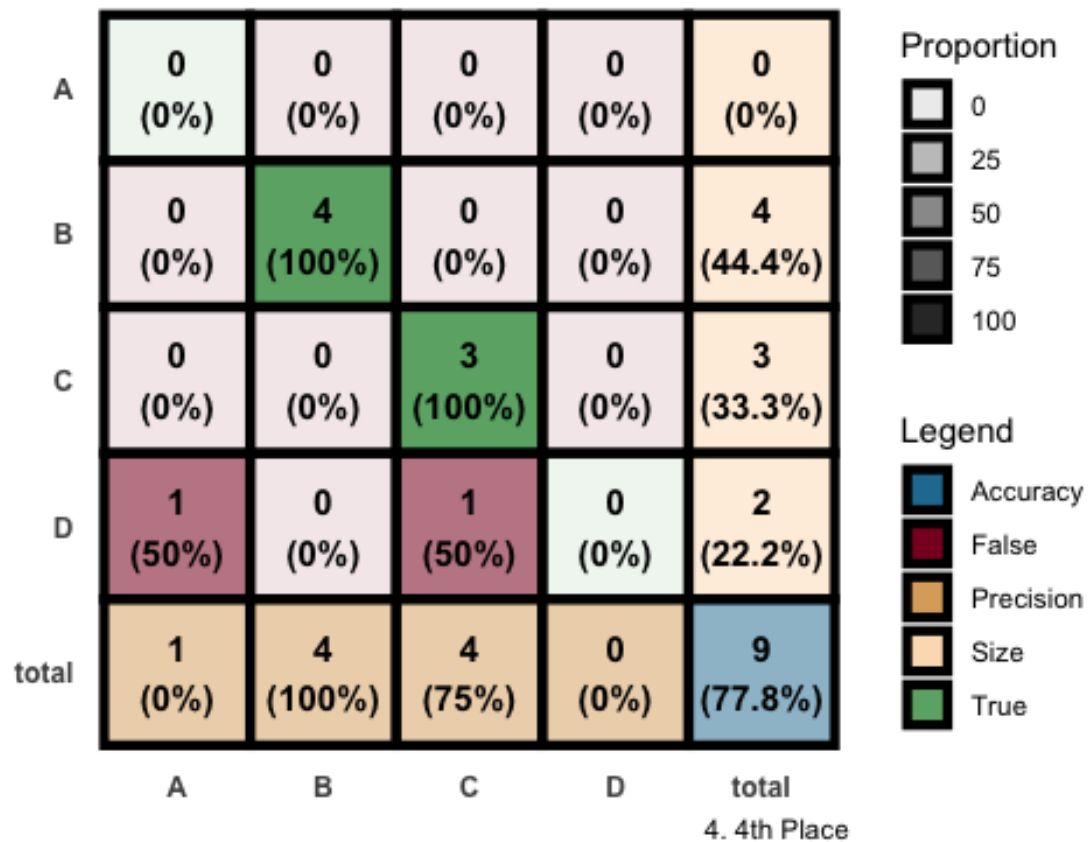
Probability Heatmap



4. 4th Place

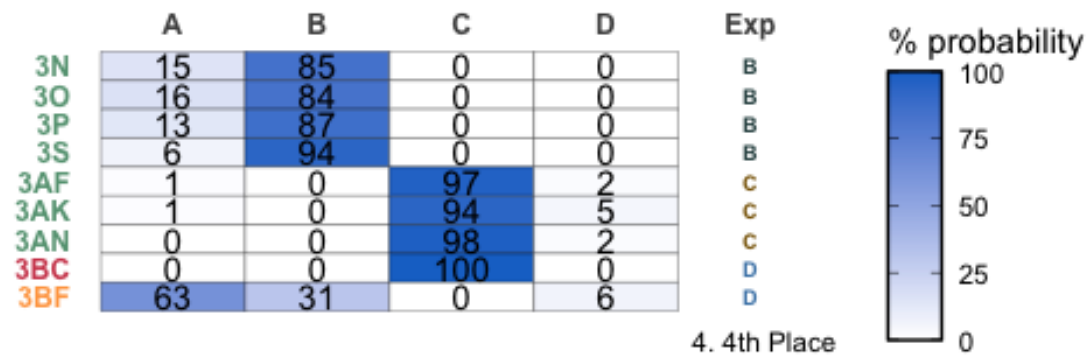
Test Set

Confusion Matrix



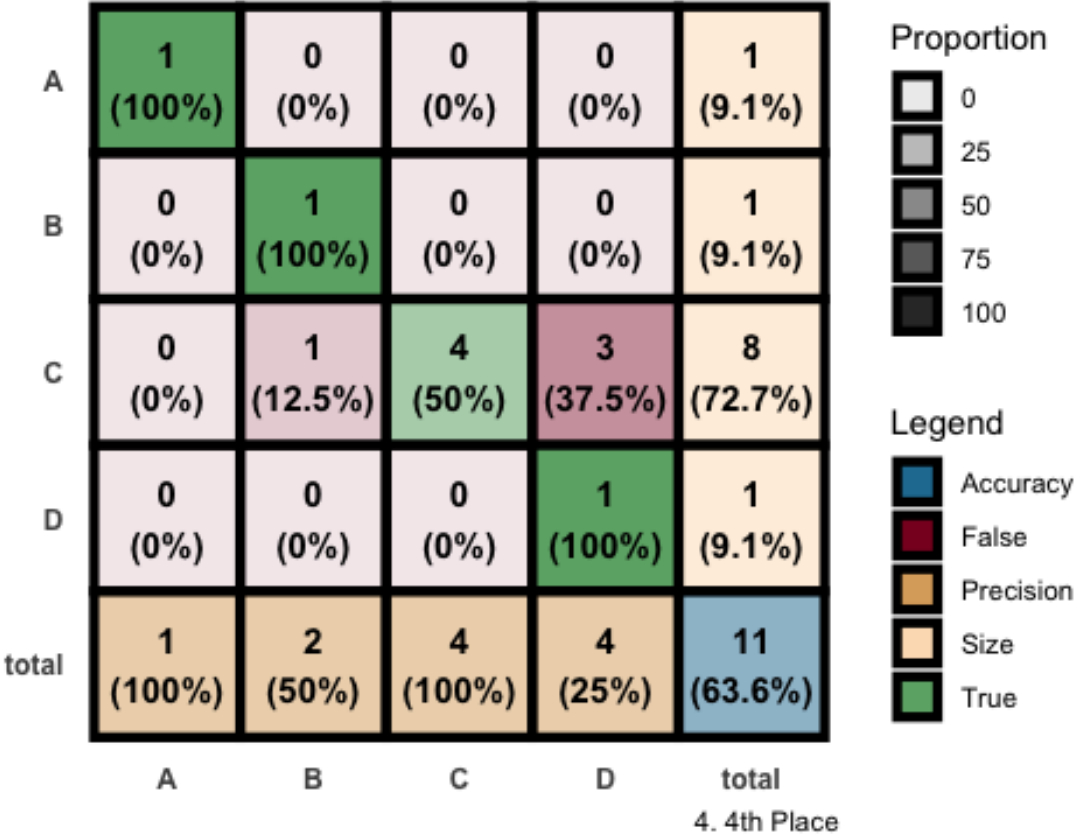
Test Set

Probability Heatmap



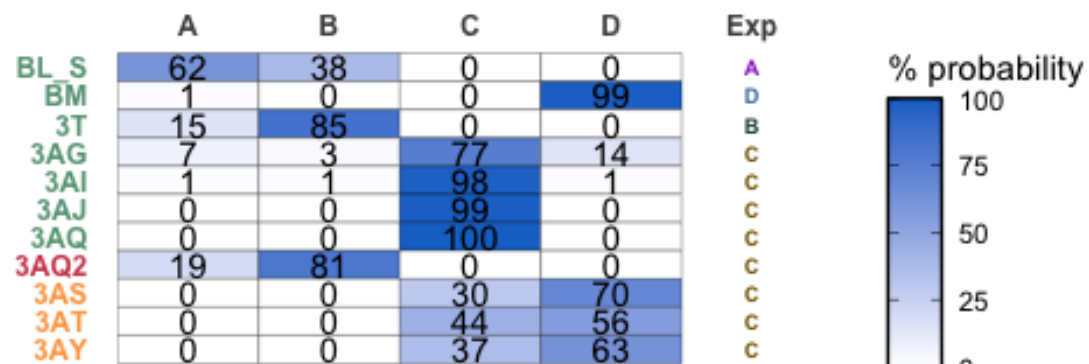
External Validation

Confusion Matrix



External Validation

Probability Heatmap



4. 4th Place

5th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

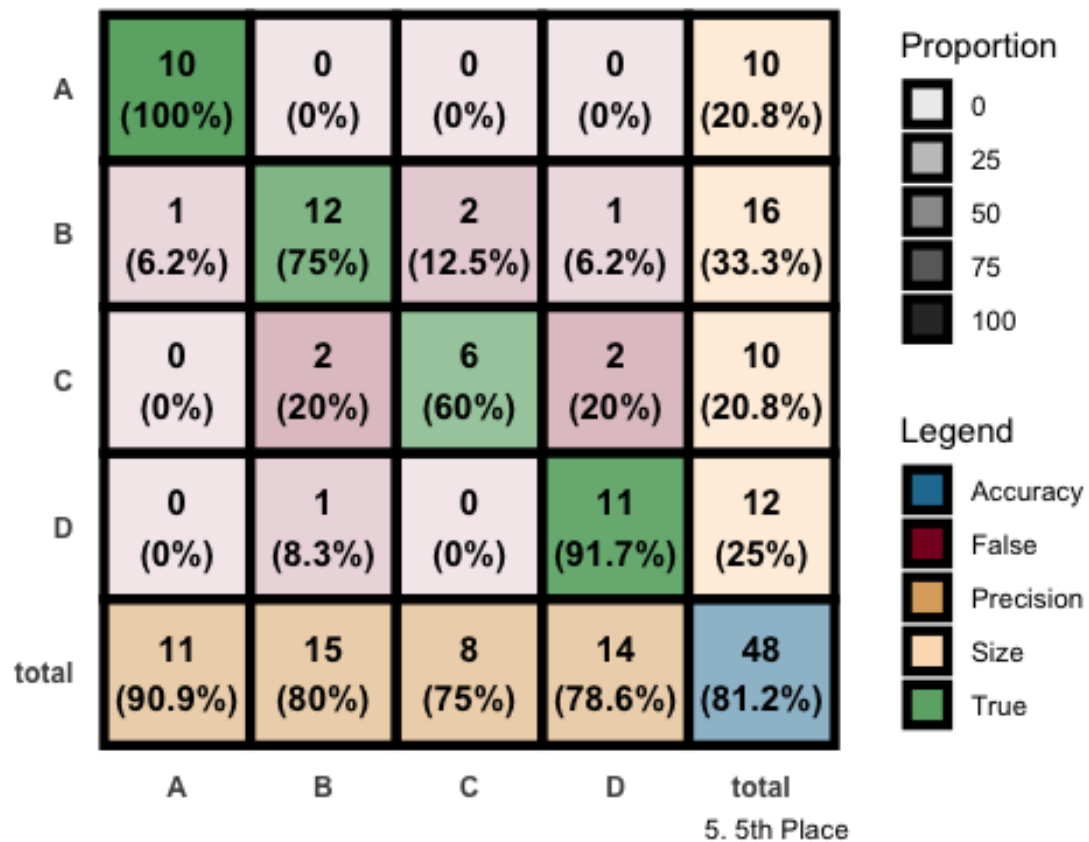
Accuracy	McFadden_R2
81.25%	0.753

Model Coefficients

	(Intercept)	NPA_13	Total_1	Dist(9, 13)	Aniso.Polar
2	209.1717	50.37315	-0.1417024	-145.4446	0.0330240
3	159.8112	55.04076	3.3328752	-106.2160	-0.1016068
4	-102.6770	31.28899	5.4790893	112.7990	-0.5154197

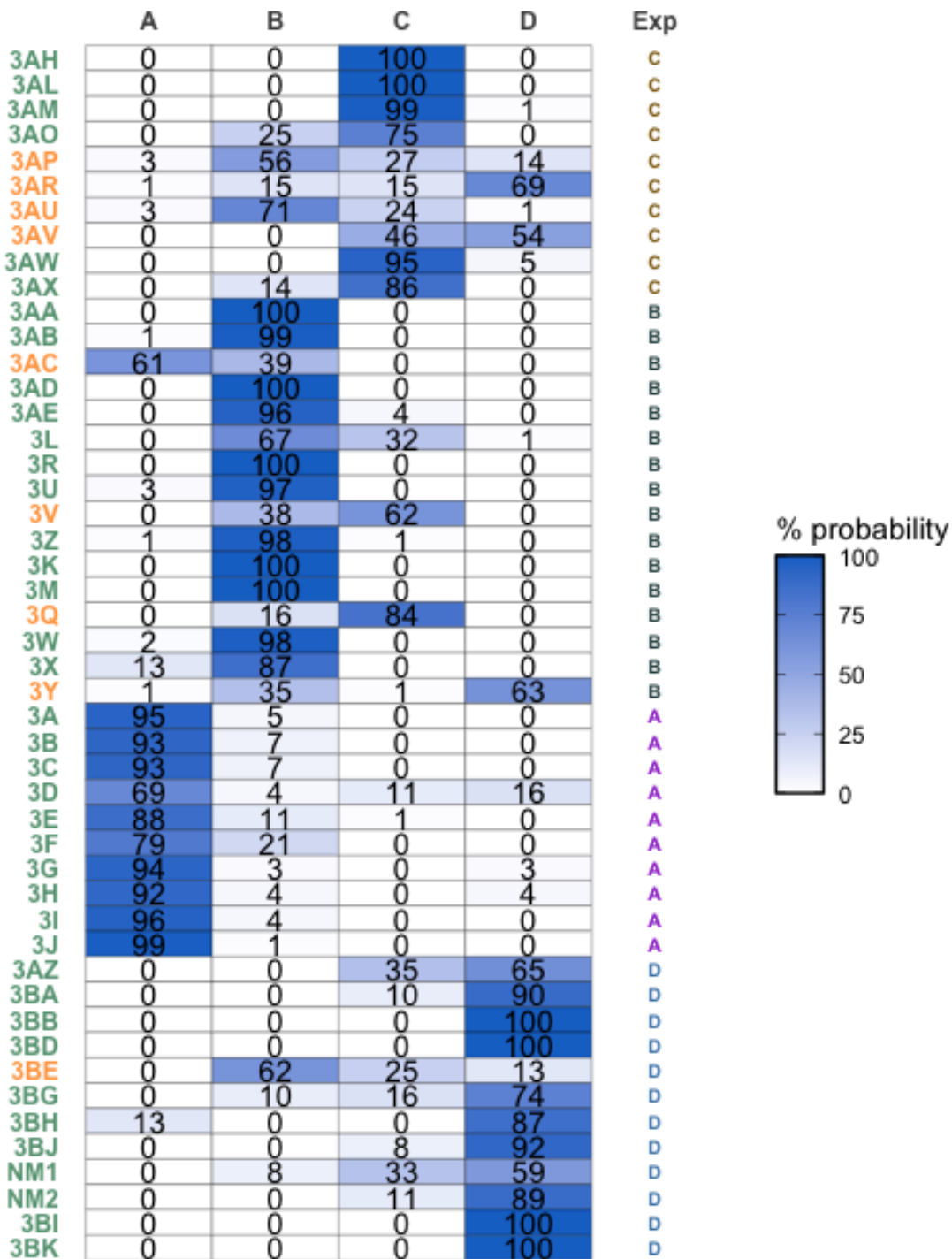
Training Set

Confusion Matrix



Training Set

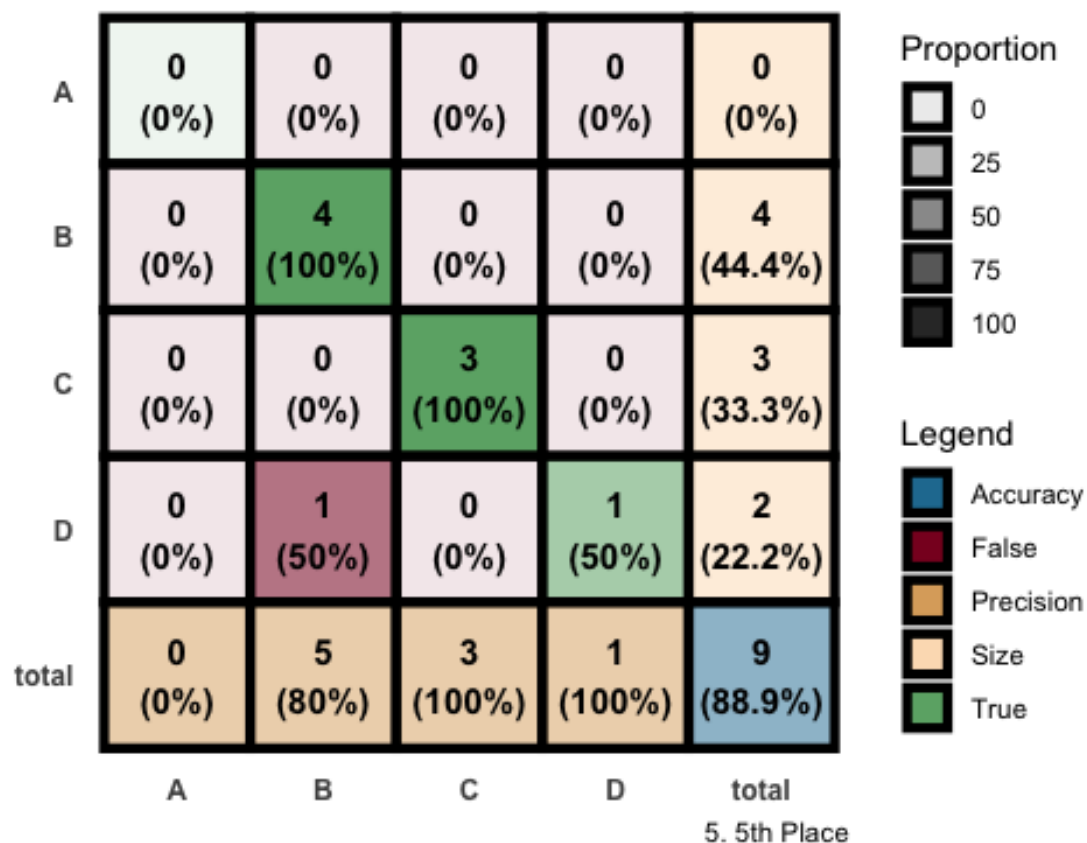
Probability Heatmap



5. 5th Place

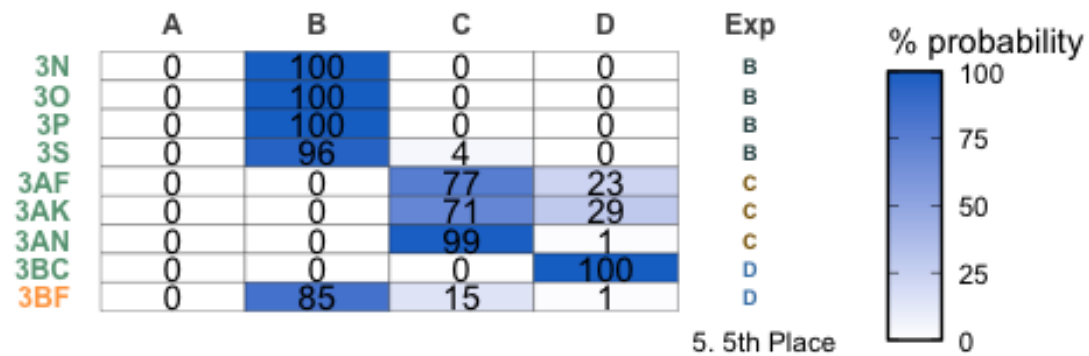
Test Set

Confusion Matrix



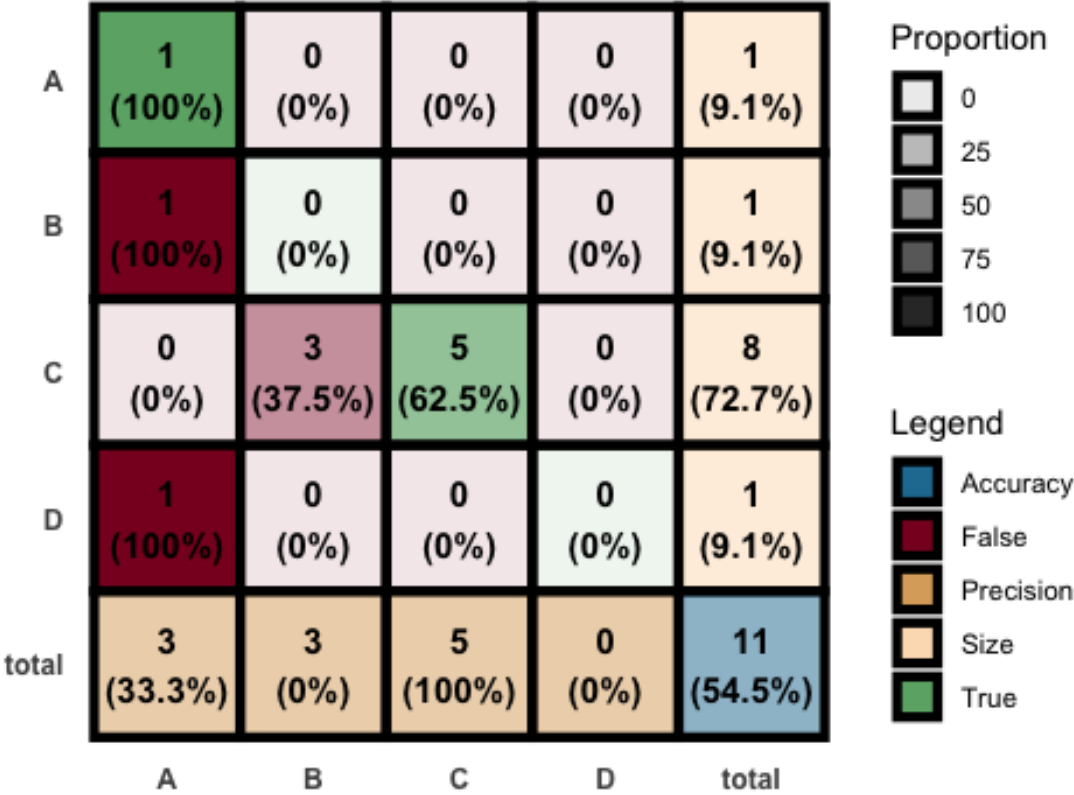
Test Set

Probability Heatmap



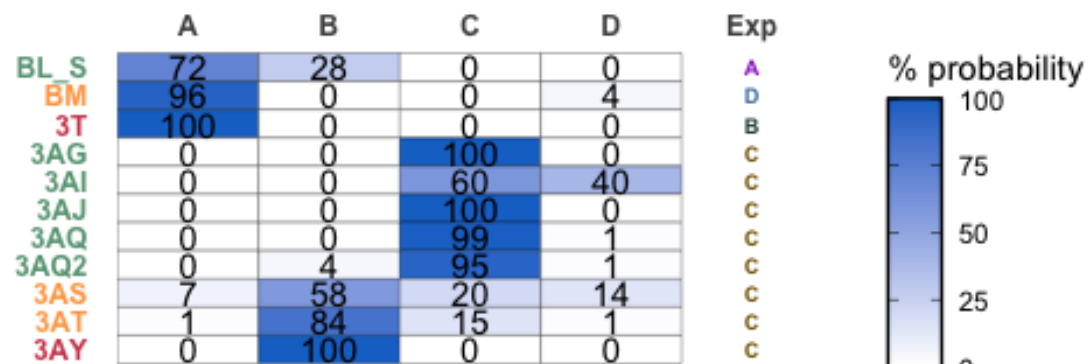
External Validation

Confusion Matrix



External Validation

Probability Heatmap



5. 5th Place

6th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
89.58%	0.753

Model Coefficients

	(Intercept)	NPA_Metallic	diff_3_4	Dist(9, 13)	Dist(3, 9)
2	253.4511	-6.16057	-13.33662	-29.92755	-146.78167
3	475.8866	-424.06029	228.44467	-496.17500	-86.58654
4	-246.2679	-19.34706	67.62215	-50.29531	199.94848

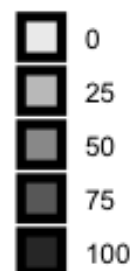
Training Set

Confusion Matrix

A	8 (80%)	1 (10%)	0 (0%)	1 (10%)	10 (20.8%)
B	1 (6.2%)	14 (87.5%)	0 (0%)	1 (6.2%)	16 (33.3%)
C	0 (0%)	0 (0%)	10 (100%)	0 (0%)	10 (20.8%)
D	0 (0%)	1 (8.3%)	0 (0%)	11 (91.7%)	12 (25%)
total	9 (88.9%)	16 (87.5%)	10 (100%)	13 (84.6%)	48 (89.6%)
	A	B	C	D	total

6. 6th Place

Proportion

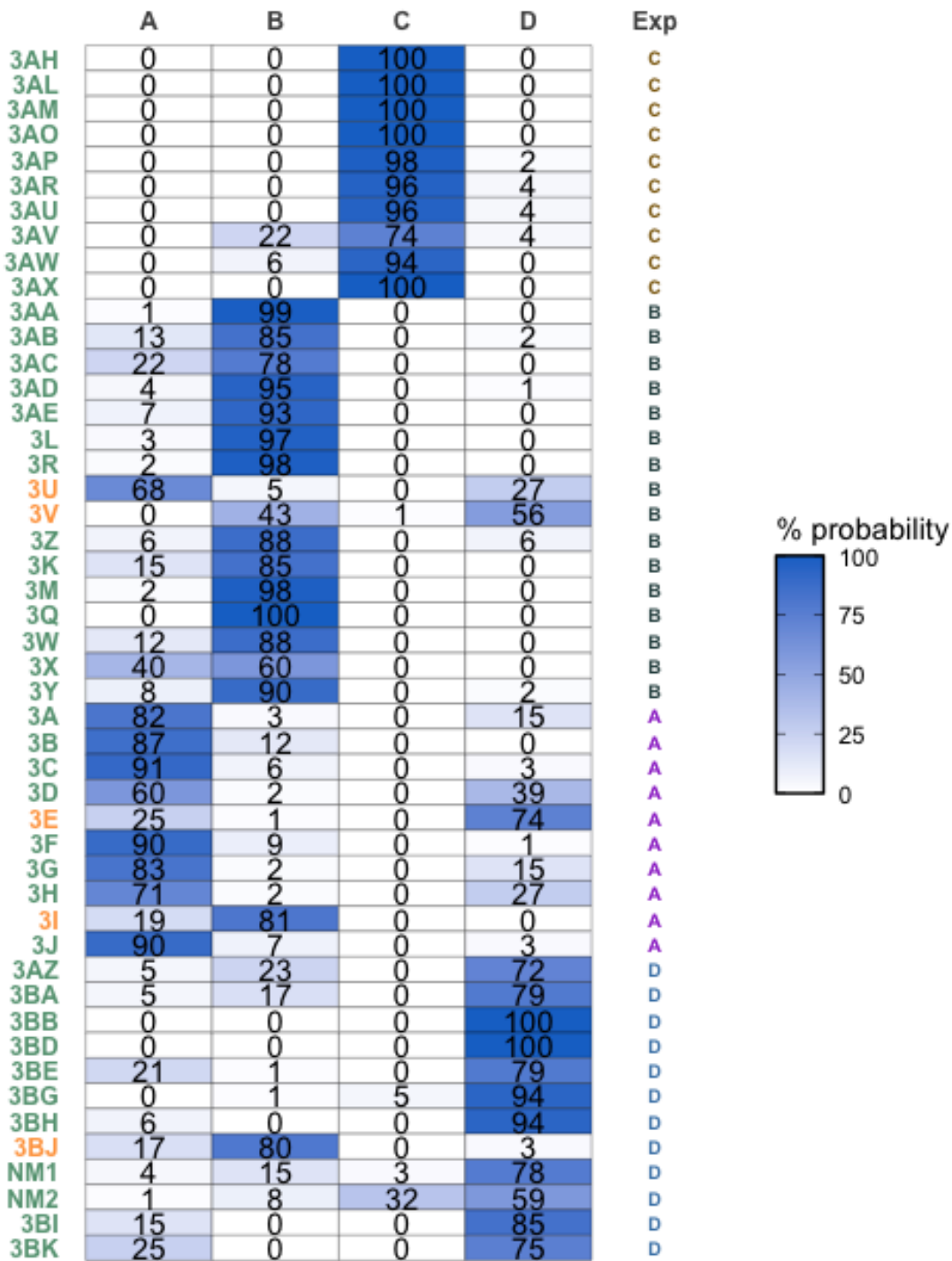


Legend



Training Set

Probability Heatmap



6. 6th Place

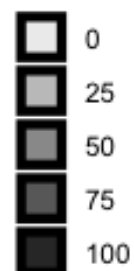
Test Set

Confusion Matrix

A	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
B	0 (0%)	4 (100%)	0 (0%)	0 (0%)	4 (44.4%)
C	0 (0%)	0 (0%)	3 (100%)	0 (0%)	3 (33.3%)
D	0 (0%)	0 (0%)	0 (0%)	2 (100%)	2 (22.2%)
total	0 (0%)	4 (100%)	3 (100%)	2 (100%)	9 (100%)
	A	B	C	D	total

6. 6th Place

Proportion

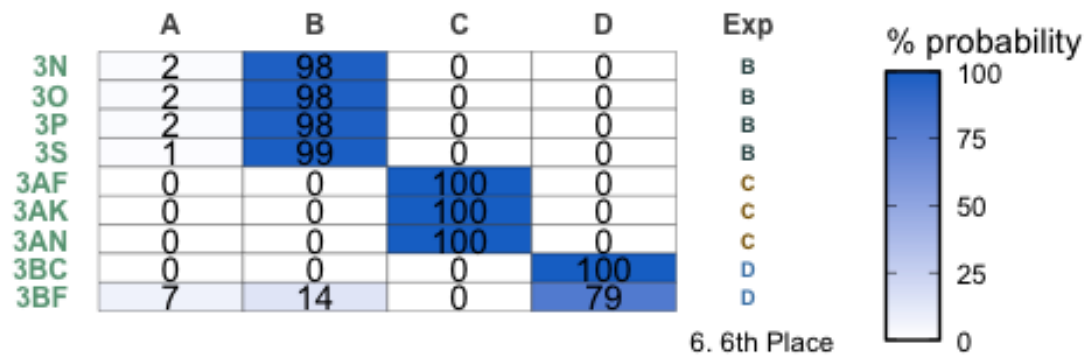


Legend



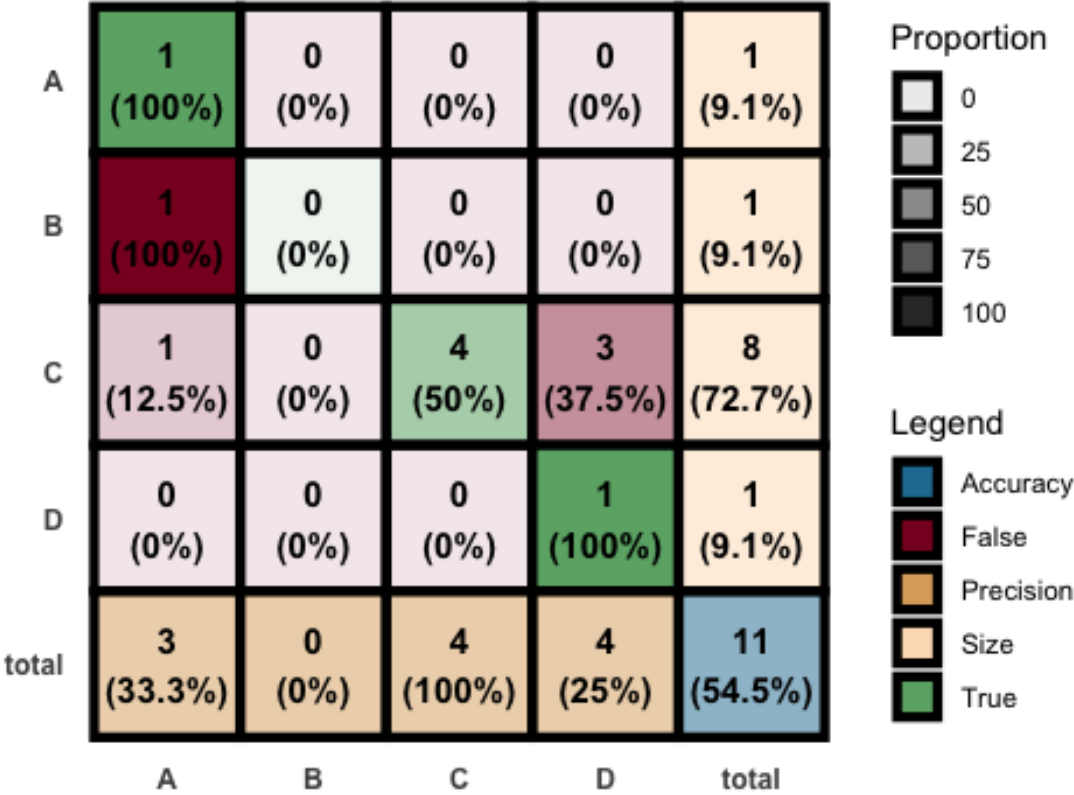
Test Set

Probability Heatmap



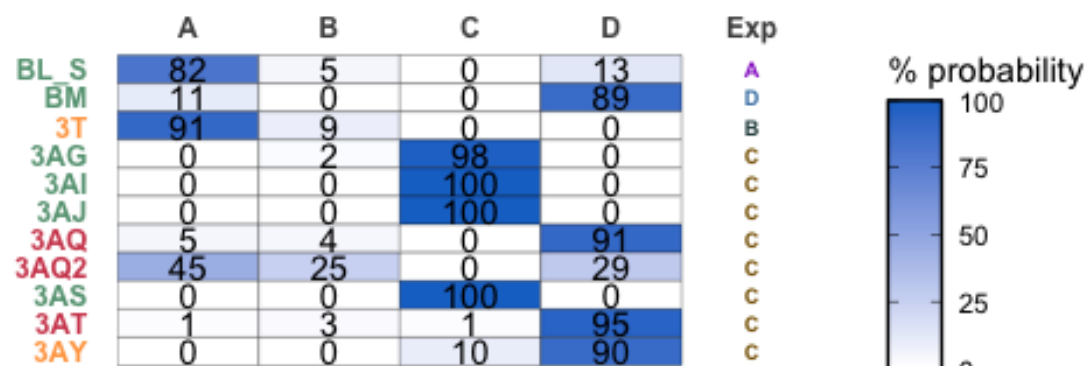
External Validation

Confusion Matrix



External Validation

Probability Heatmap



6. 6th Place

7th Place

Table:

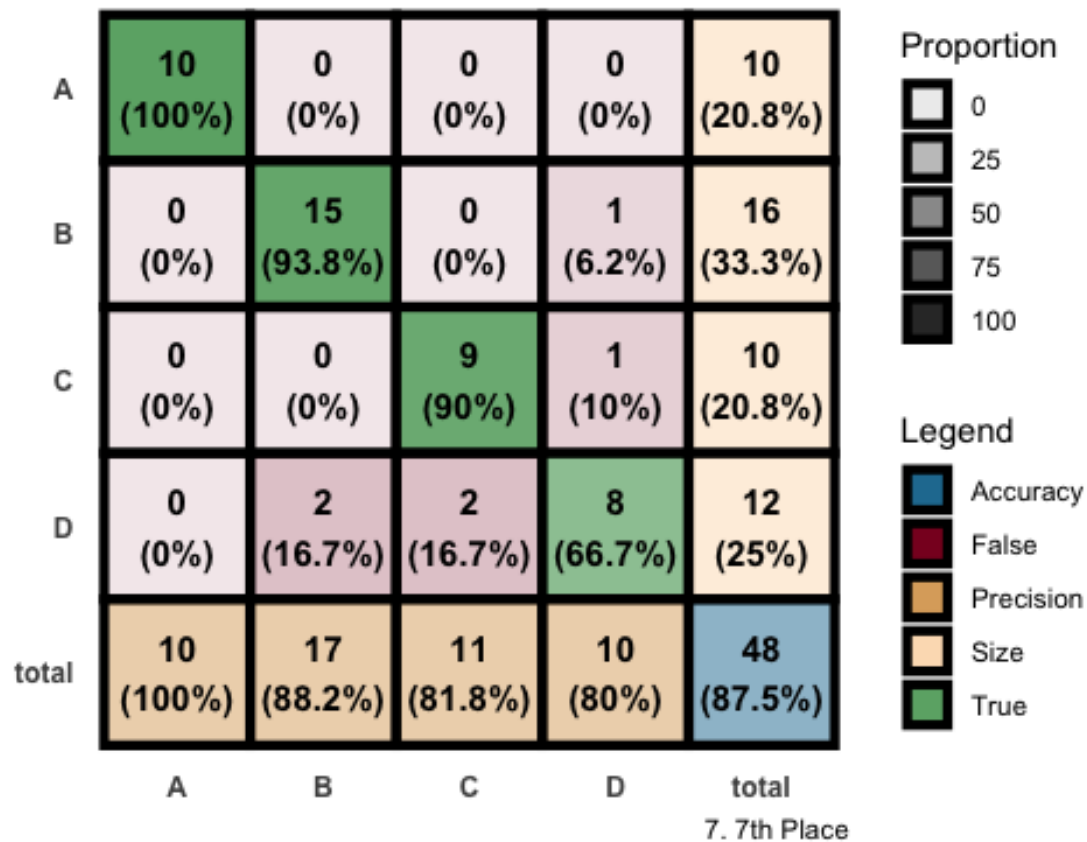
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
87.5%	0.75

Model Coefficients

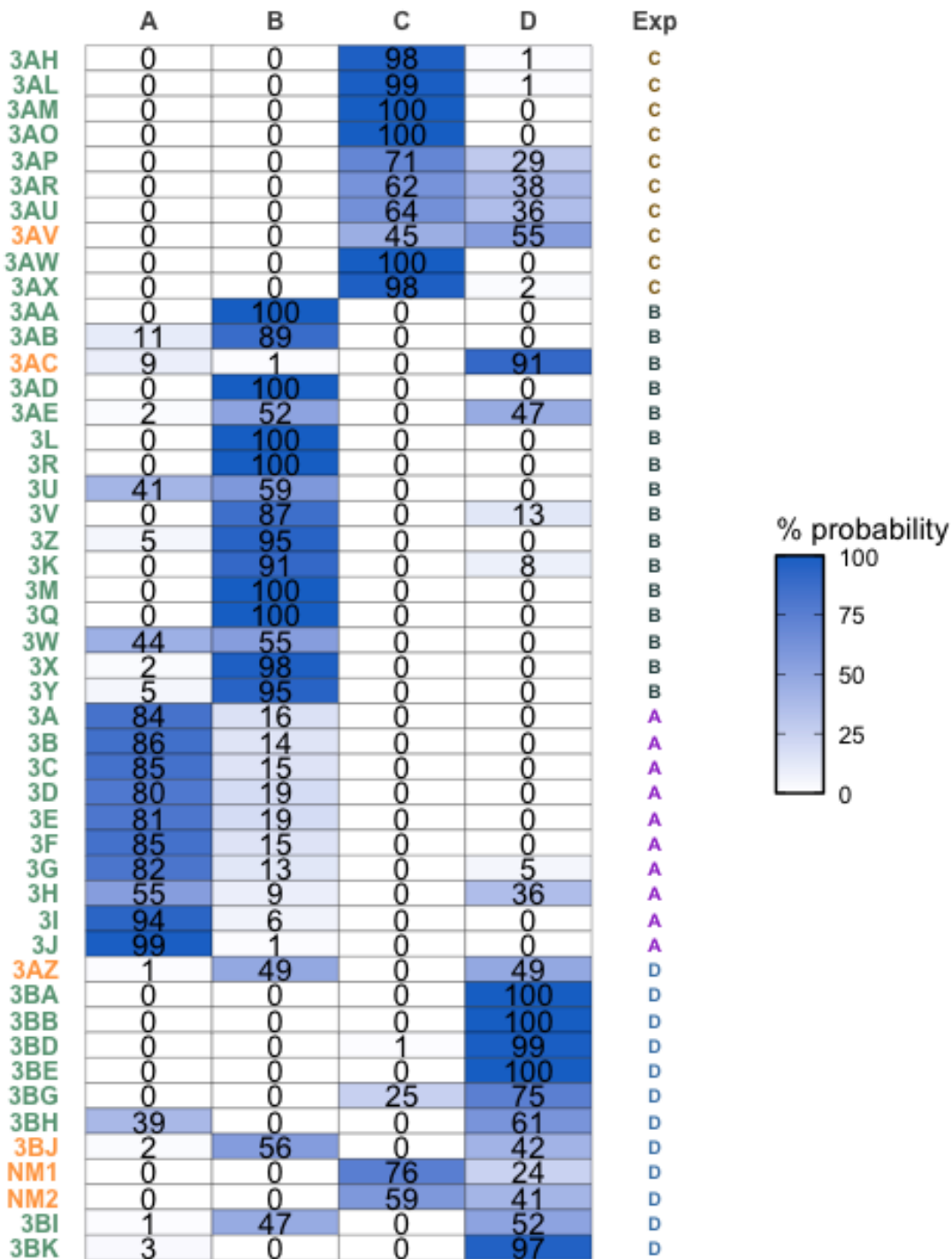
	(Intercept)	B1_2	diff_9_13	diff_10_Metalla	Dist(9, 13)
2	125.180332	-0.0134859	-14.173455	13.83981	-95.32624
3	-3.895553	34.9206666	-18.616192	271.36109	-207.84260
4	-90.416980	31.8120948	-7.791345	136.17444	-48.39899

Training Set Confusion Matrix



Training Set

Probability Heatmap



7. 7th Place

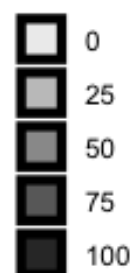
Test Set

Confusion Matrix

A	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
B	0 (0%)	4 (100%)	0 (0%)	0 (0%)	4 (44.4%)
C	0 (0%)	0 (0%)	3 (100%)	0 (0%)	3 (33.3%)
D	0 (0%)	0 (0%)	0 (0%)	2 (100%)	2 (22.2%)
total	0 (0%)	4 (100%)	3 (100%)	2 (100%)	9 (100%)
	A	B	C	D	total

7. 7th Place

Proportion

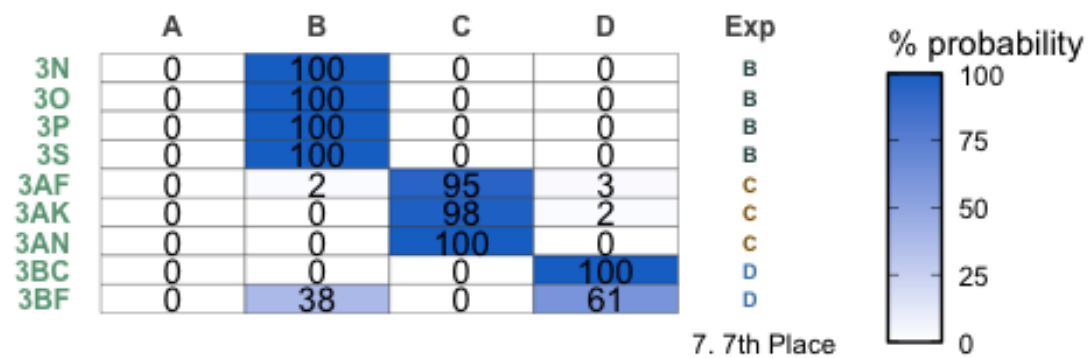


Legend



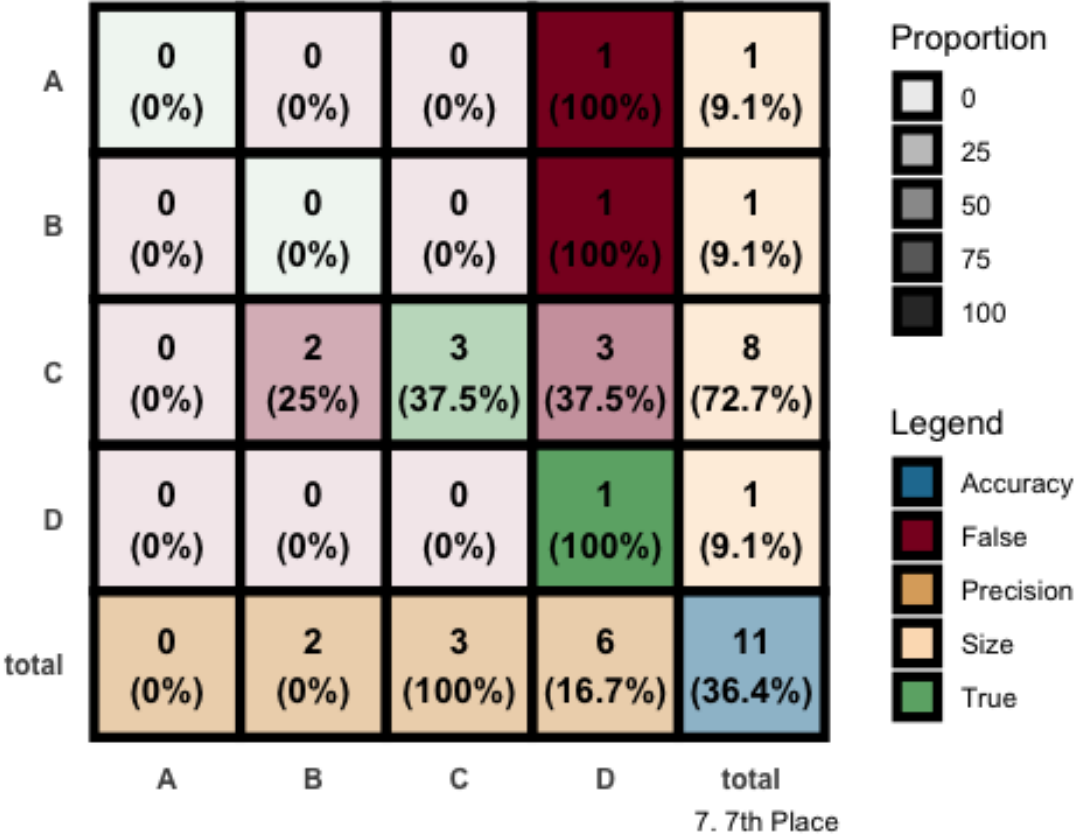
Test Set

Probability Heatmap



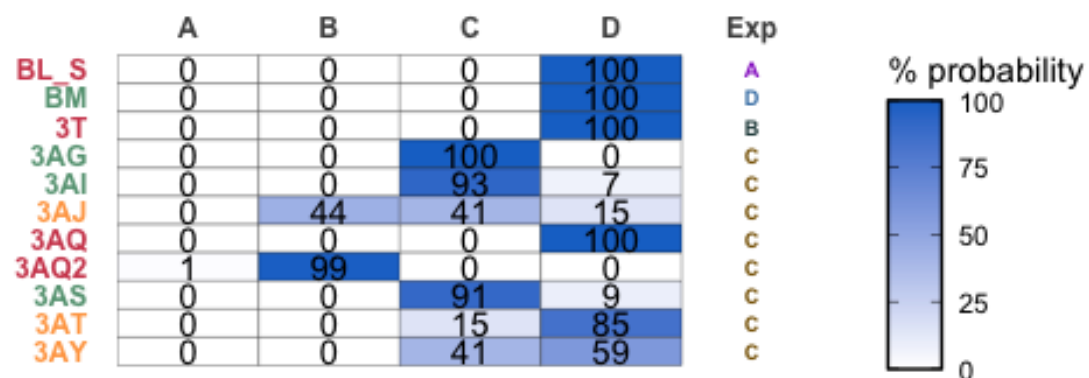
External Validation

Confusion Matrix



External Validation

Probability Heatmap



7. 7th Place

8th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

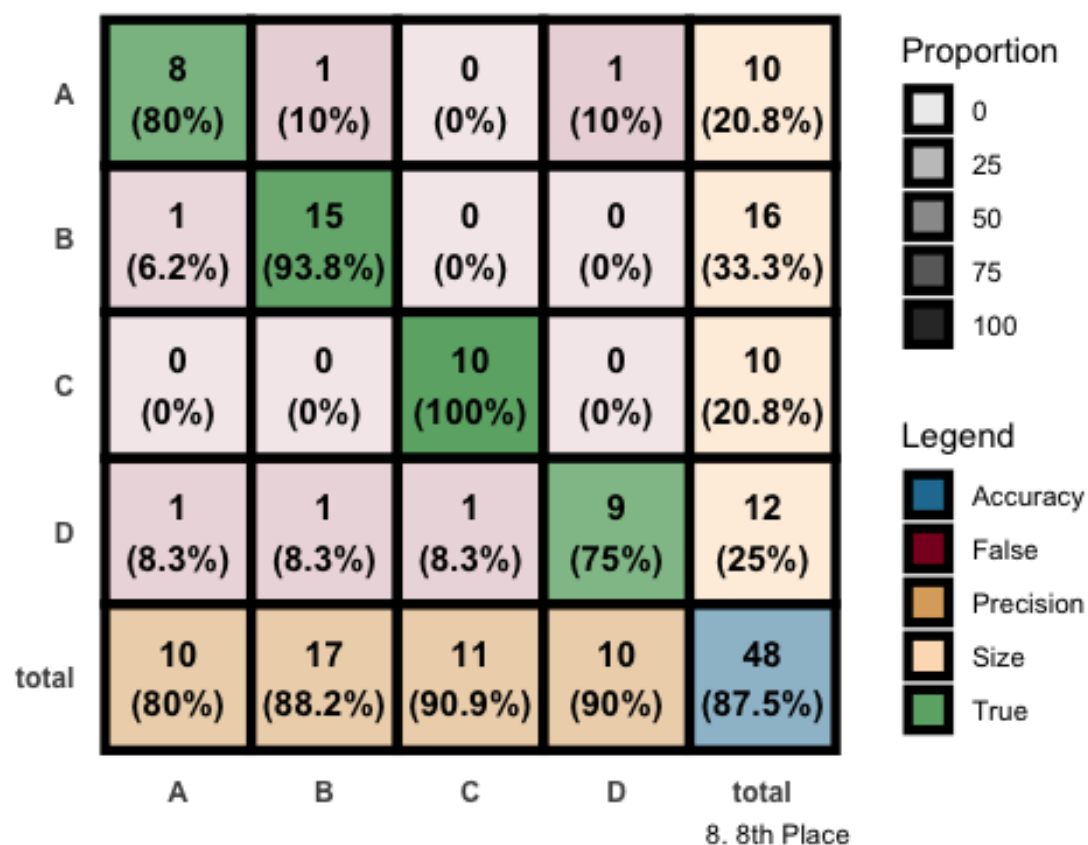
Accuracy	McFadden_R2
87.5%	0.749

Model Coefficients

	(Intercept)	B1_1	NPA_13	diff_10_Metalla	Dist(9, 13)
2	182.41905	-11.75716	35.59387	-42.67848	-88.90331
3	227.52047	31.96499	70.92215	393.40179	-471.29971
4	-35.44666	12.59796	16.95644	54.00225	-15.81256

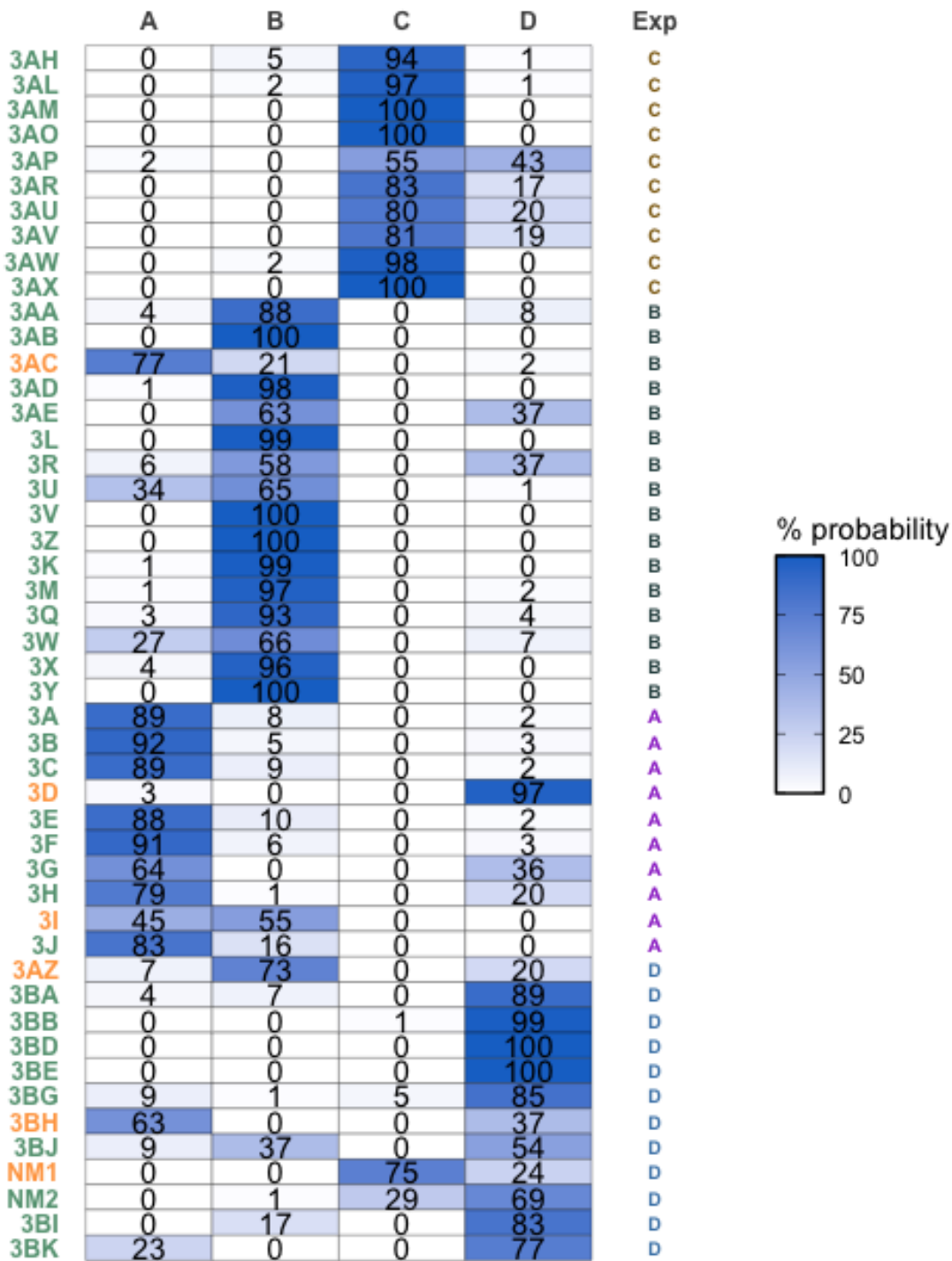
Training Set

Confusion Matrix



Training Set

Probability Heatmap



8. 8th Place

Test Set

Confusion Matrix

A	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
B	0 (0%)	2 (50%)	0 (0%)	2 (50%)	4 (44.4%)
C	0 (0%)	2 (66.7%)	1 (33.3%)	0 (0%)	3 (33.3%)
D	0 (0%)	1 (50%)	1 (50%)	0 (0%)	2 (22.2%)
total	0 (0%)	5 (40%)	2 (50%)	2 (0%)	9 (33.3%)
	A	B	C	D	total

Legend

- Accuracy
- False
- Precision
- Size
- True

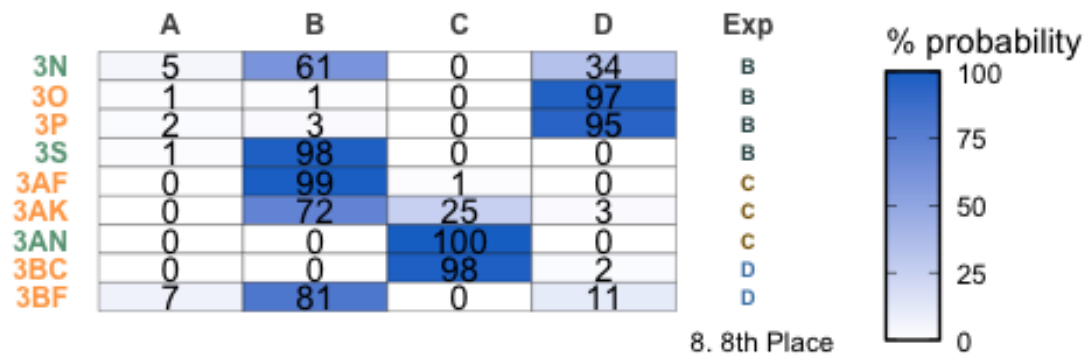
Proportion

- 0
- 20
- 40
- 60

8. 8th Place

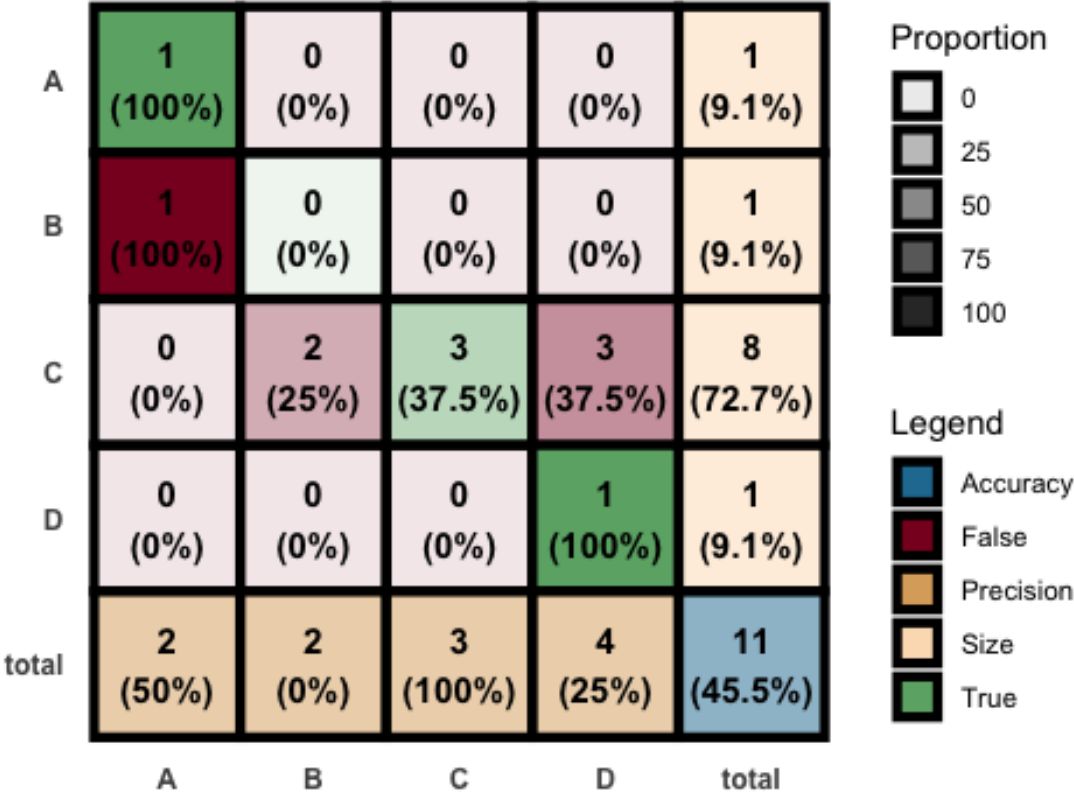
Test Set

Probability Heatmap



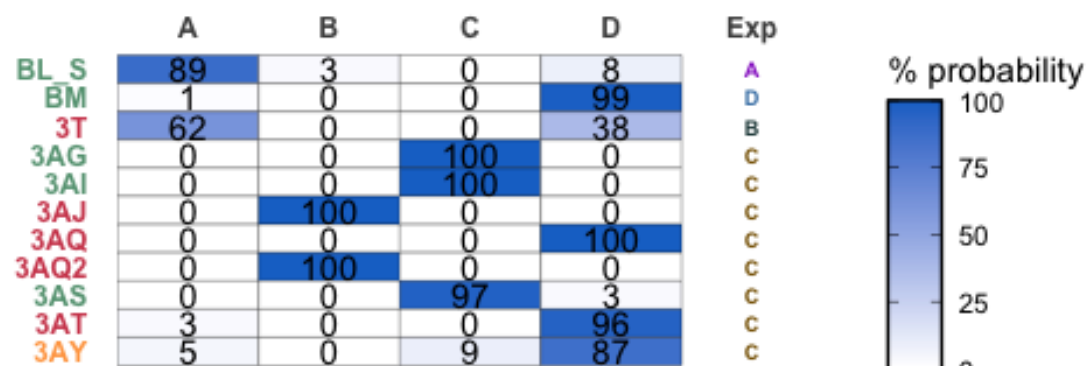
External Validation

Confusion Matrix



External Validation

Probability Heatmap



8. 8th Place

9th Place

Table:

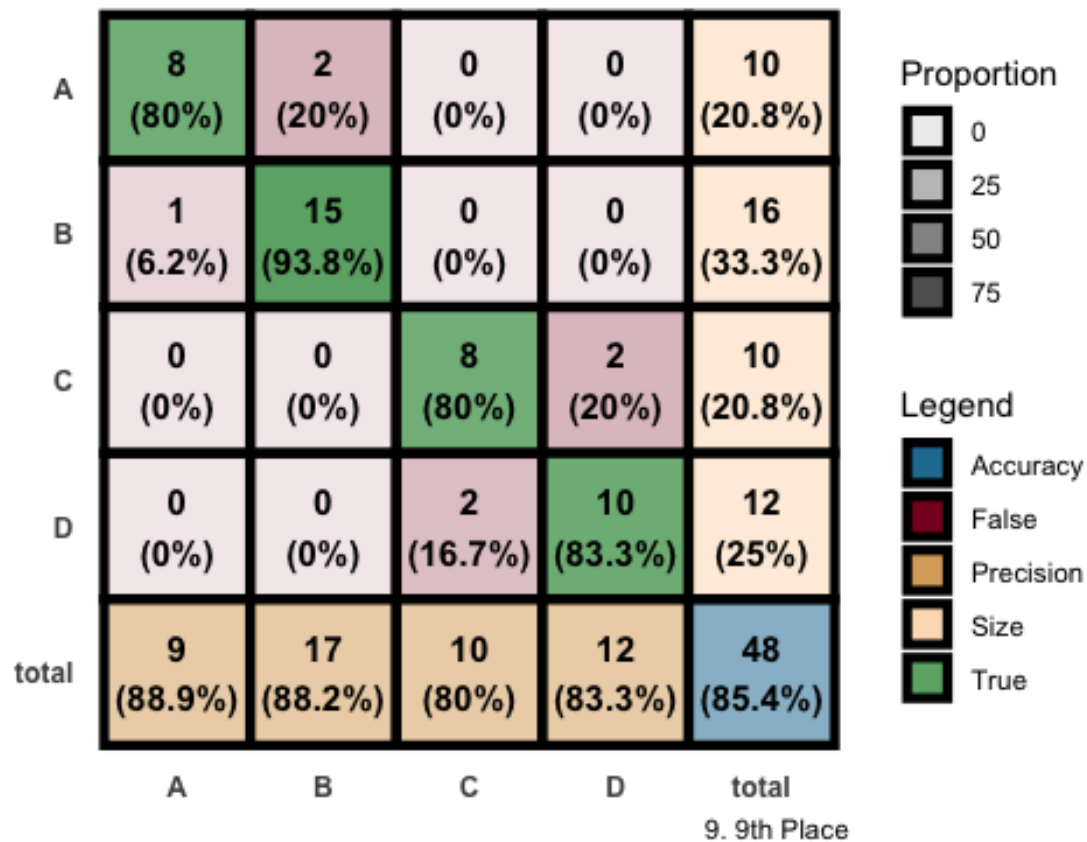
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
85.42%	0.749

Model Coefficients

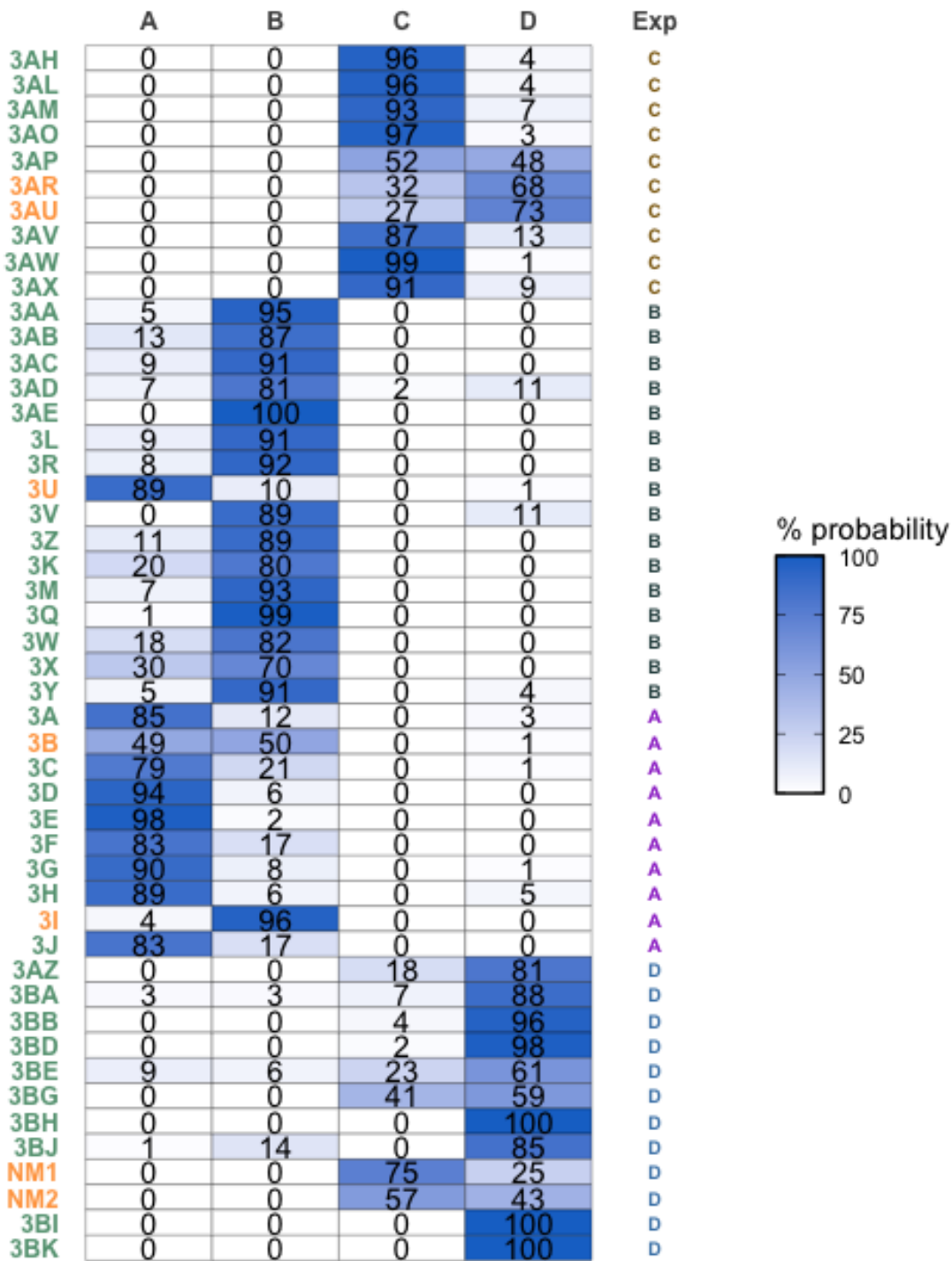
	(Intercept)	diff_3_4	diff_10_Metalla	dip_y_1	Dist(3, 9)
2	215.9409	-16.83978	10.26633	-0.3283084	-150.3181
3	-372.3417	83.18818	84.59903	-4.0670111	197.0228
4	-444.9479	95.36234	40.46084	-3.5037489	271.4785

Training Set Confusion Matrix



Training Set

Probability Heatmap



9. 9th Place

Test Set

Confusion Matrix

A	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
B	0 (0%)	4 (100%)	0 (0%)	0 (0%)	4 (44.4%)
C	0 (0%)	0 (0%)	3 (100%)	0 (0%)	3 (33.3%)
D	0 (0%)	0 (0%)	0 (0%)	2 (100%)	2 (22.2%)
total	0 (0%)	4 (100%)	3 (100%)	2 (100%)	9 (100%)
	A	B	C	D	total

Proportion



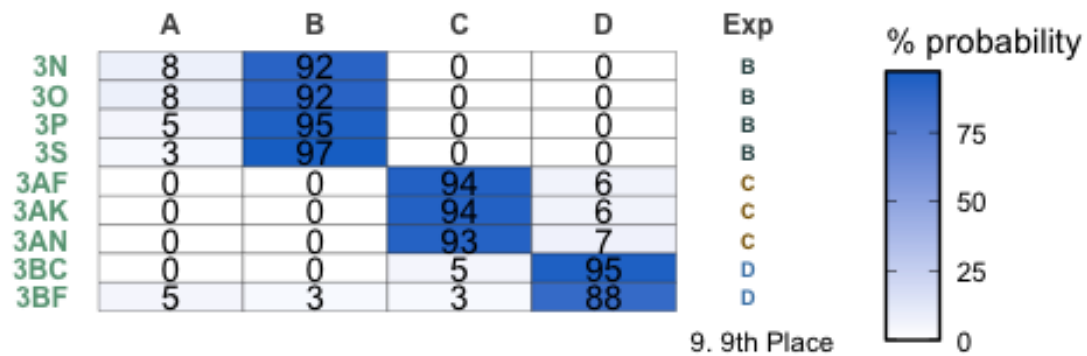
Legend



9. 9th Place

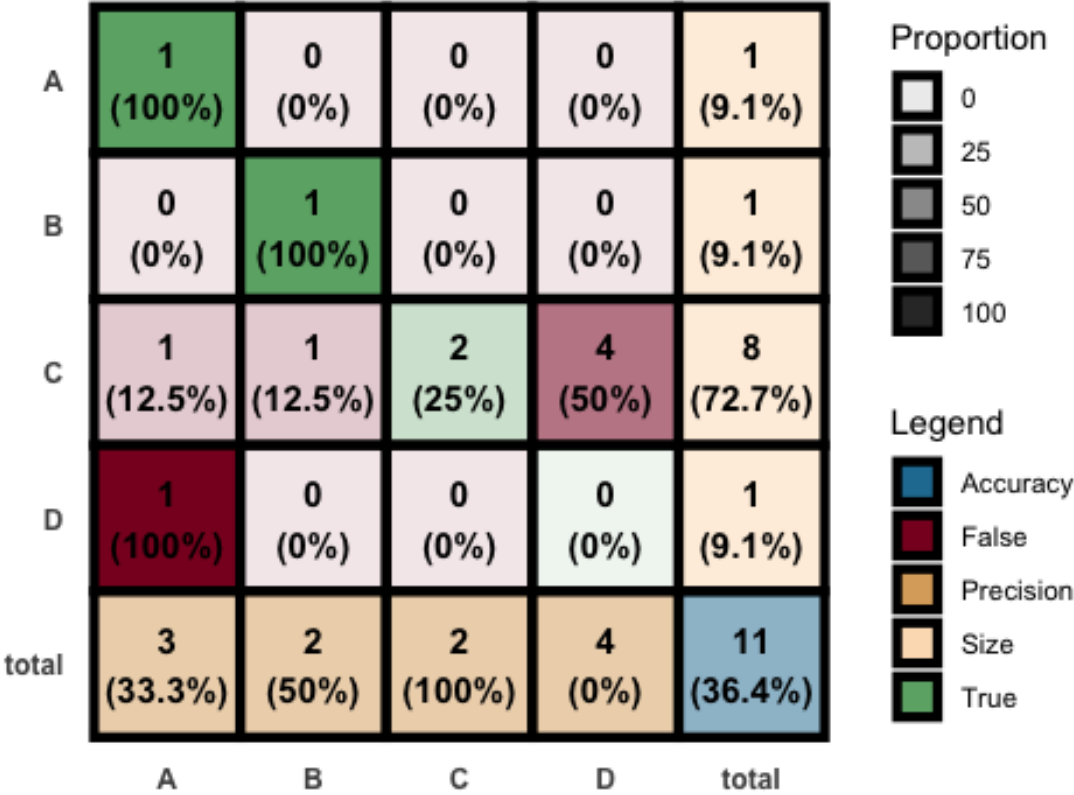
Test Set

Probability Heatmap



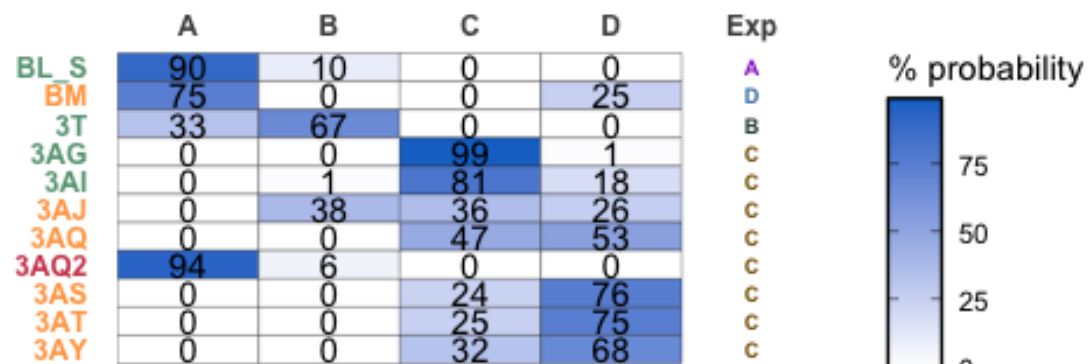
External Validation

Confusion Matrix



External Validation

Probability Heatmap



9. 9th Place

10th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
89.58%	0.748

Model Coefficients

	(Intercept)	B1_2	NPA_13	diff_10_Metalla	Dist(9, 13)
2	122.00046	-2.267609	30.04532	-7.978693	-76.08444
3	45.63427	31.897558	46.45992	290.148854	-254.84863
4	-96.10339	28.516278	18.04905	122.536861	-29.82083

Training Set Confusion Matrix

A	10 (100%)	0 (0%)	0 (0%)	0 (0%)	10 (20.8%)
B	0 (0%)	15 (93.8%)	0 (0%)	1 (6.2%)	16 (33.3%)
C	0 (0%)	0 (0%)	10 (100%)	0 (0%)	10 (20.8%)
D	0 (0%)	2 (16.7%)	2 (16.7%)	8 (66.7%)	12 (25%)
total	10 (100%)	17 (88.2%)	12 (83.3%)	9 (88.9%)	48 (89.6%)
	A	B	C	D	total

Proportion

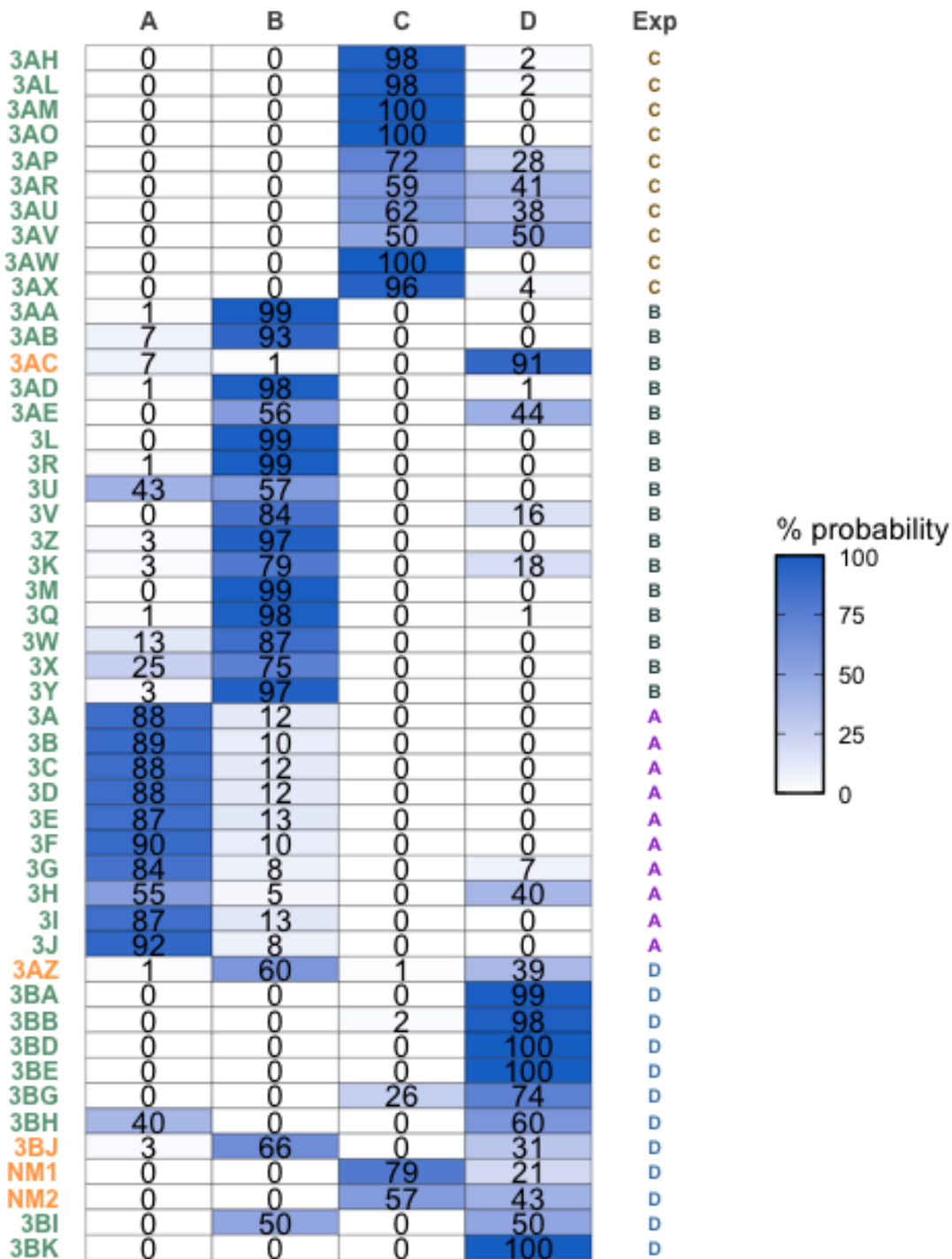


Legend



Training Set

Probability Heatmap



10. 10th Place

Test Set

Confusion Matrix

A	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
B	0 (0%)	4 (100%)	0 (0%)	0 (0%)	4 (44.4%)
C	0 (0%)	0 (0%)	3 (100%)	0 (0%)	3 (33.3%)
D	0 (0%)	0 (0%)	0 (0%)	2 (100%)	2 (22.2%)
total	0 (0%)	4 (100%)	3 (100%)	2 (100%)	9 (100%)
	A	B	C	D	total

Proportion

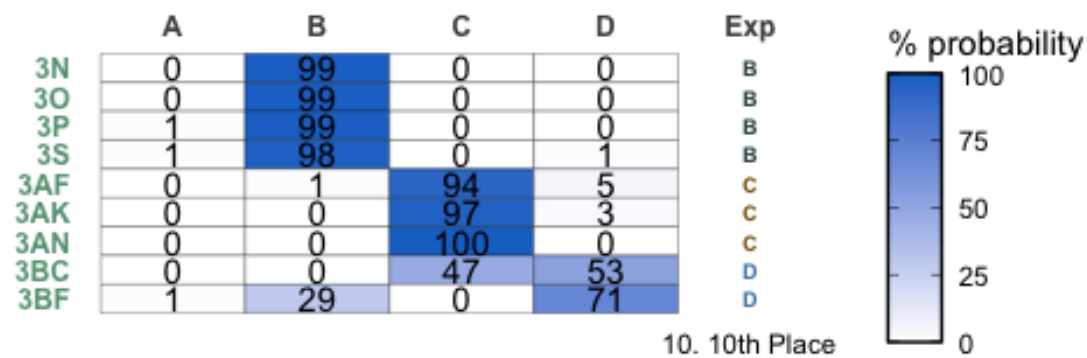


Legend



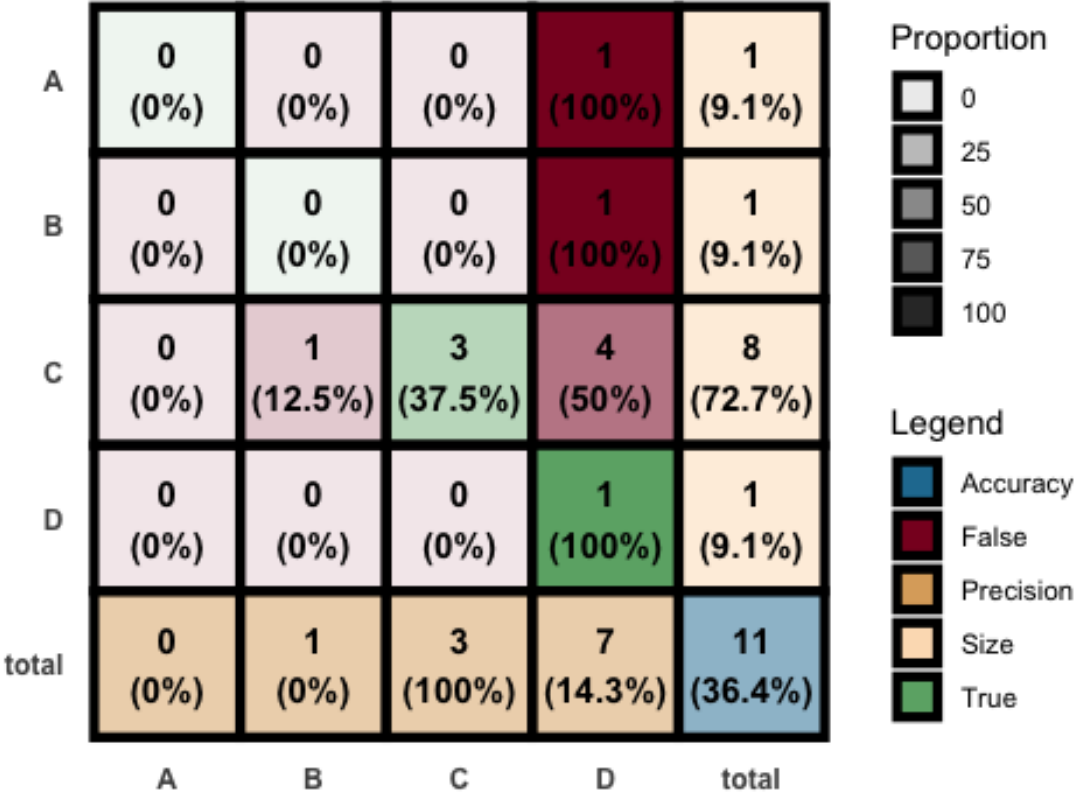
Test Set

Probability Heatmap



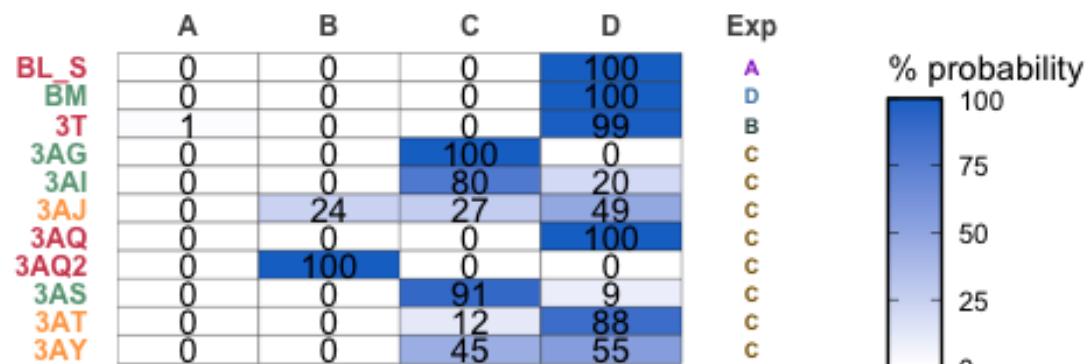
External Validation

Confusion Matrix



External Validation

Probability Heatmap



10. 10th Place