

Aldehyde Deuteration - Model Search - Full sets, non-ordinal

Model Search

formula	McFadden R2
class ~ -2-3- + dip_x + dip_y + NPA_1	0.729
class ~ -2-3- + dip_x + dip_y + diff 1 2	0.729
class ~ dip_x + dip_y + Dist(2, 3) + NPA_1	0.709
class ~ dip_x + dip_y + NPA_3 + diff 1 2	0.708
class ~ dip_y + NPA_3 + diff 1 2 + loc.B5	0.704
class ~ dip_x + dip_y + Dist(2, 3) + diff 1 2	0.703
class ~ dip_x + dip_y + NPA_1 + NPA_3	0.702
class ~ dip_x + dip_y + NPA_1 + loc.B5	0.693
class ~ Total + NPA_1 + diff 2 3 + loc.B5	0.690
class ~ dip_y + NPA_1 + NPA_3 + loc.B5	0.689

1st Place

Table:

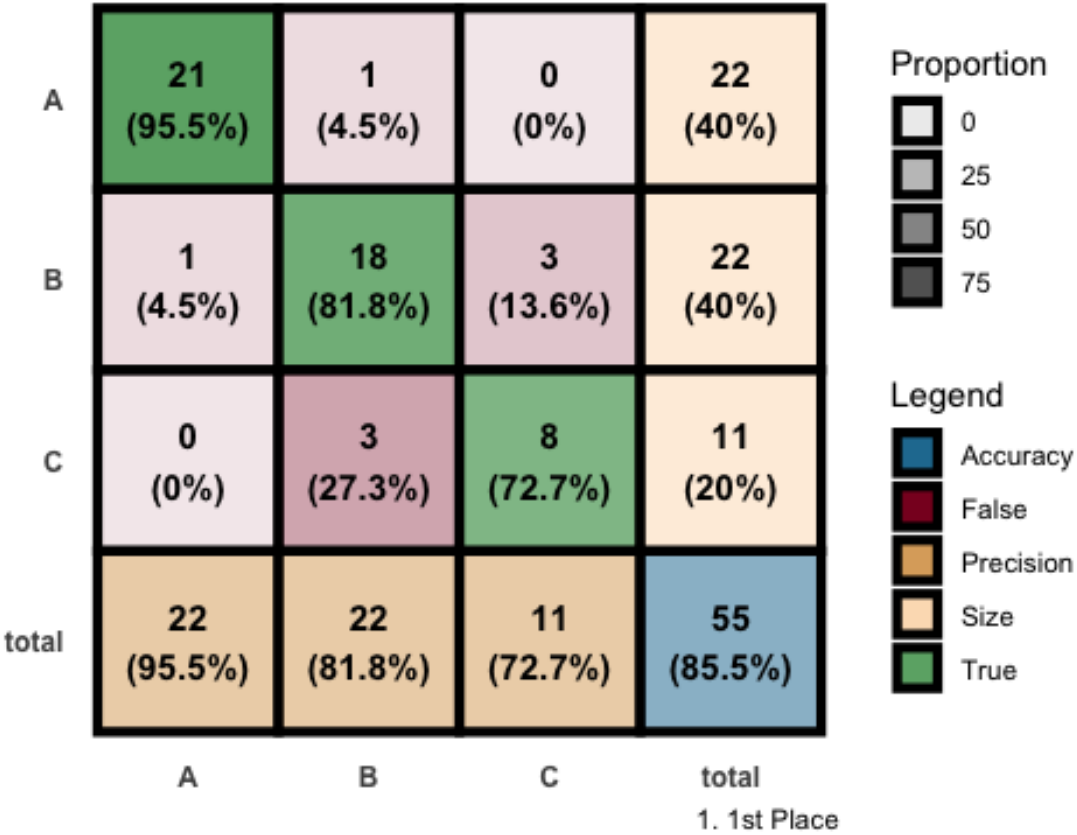
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
85.45%	0.729

Model Coefficients

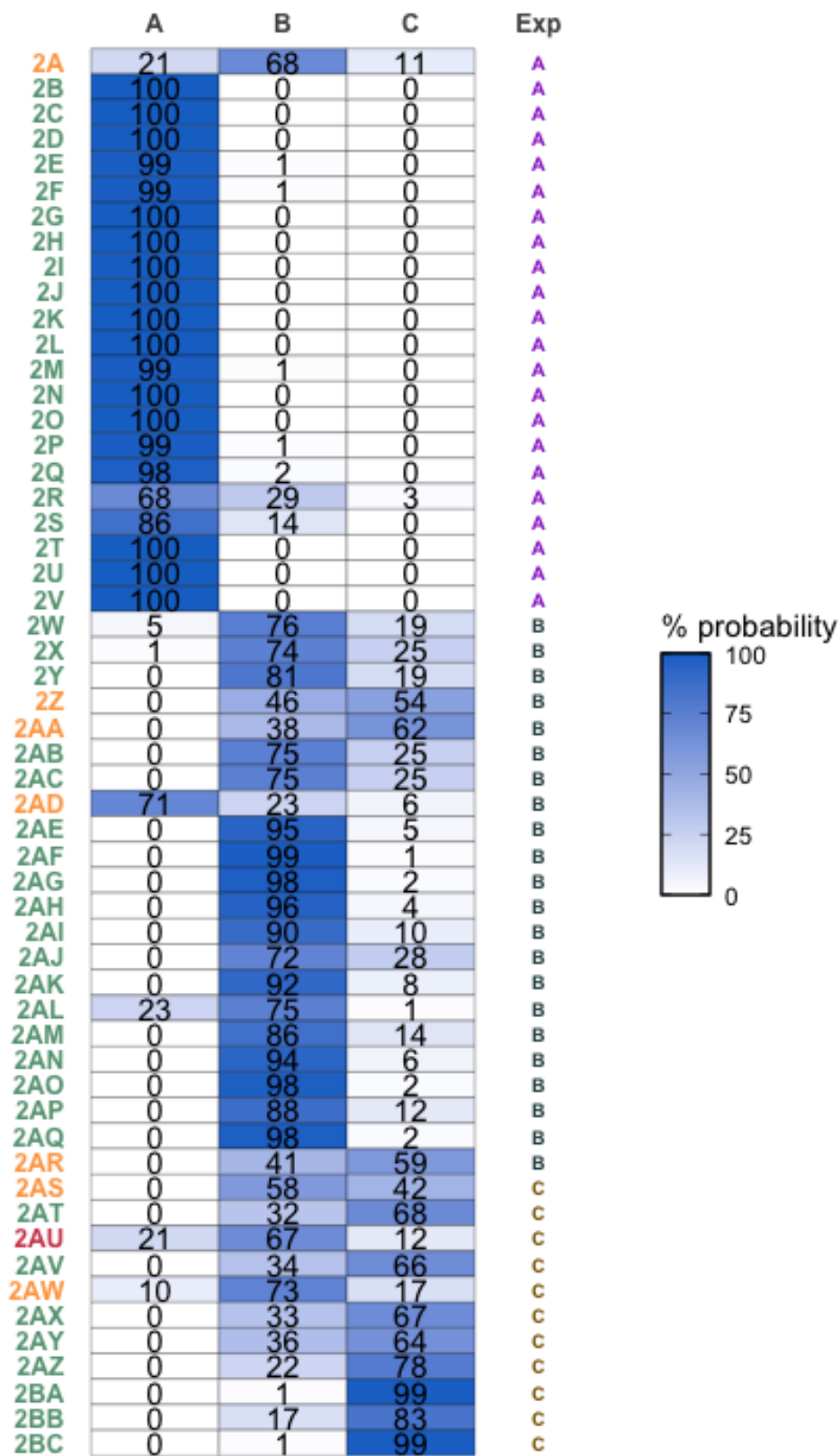
	(Intercept)	-2-3-	dip_x	dip_y	NPA_1
2	-215.4406	0.1111802	-9.125786	-13.75496	153.4555
3	239.9362	-0.1378071	-8.924340	-14.52949	166.4614

Training Set
Confusion Matrix



Training Set

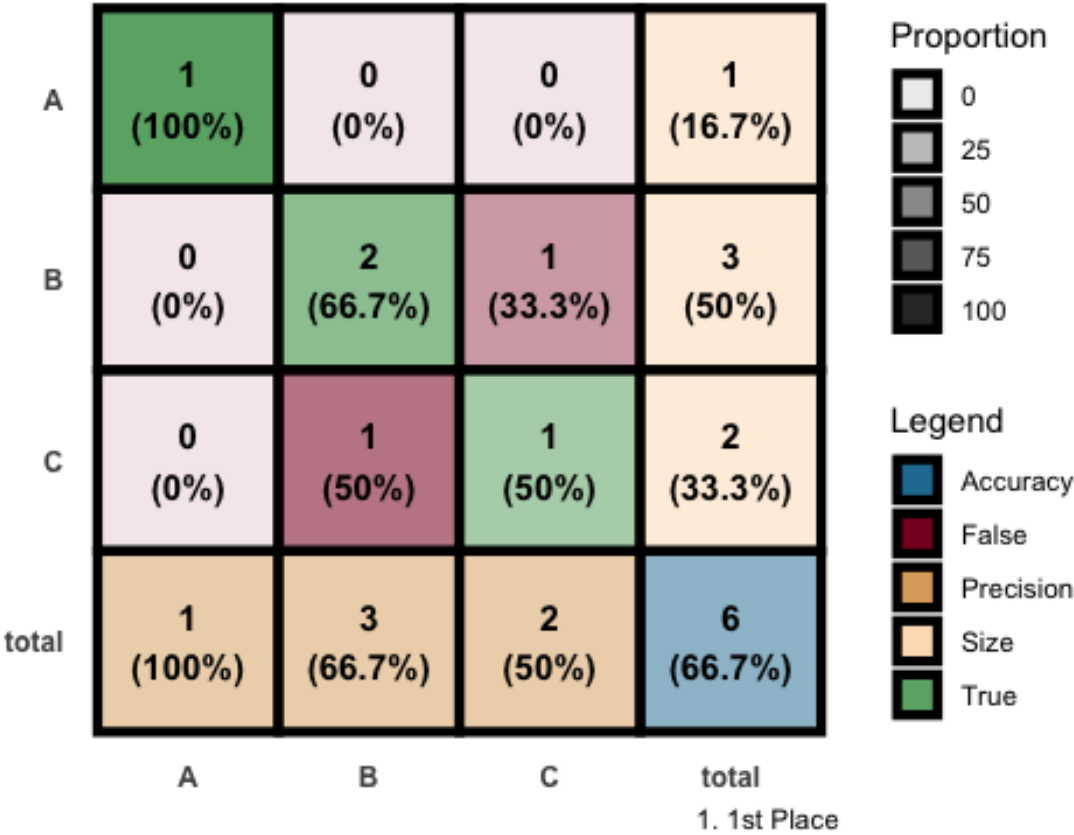
Probability Heatmap



1. 1st Place

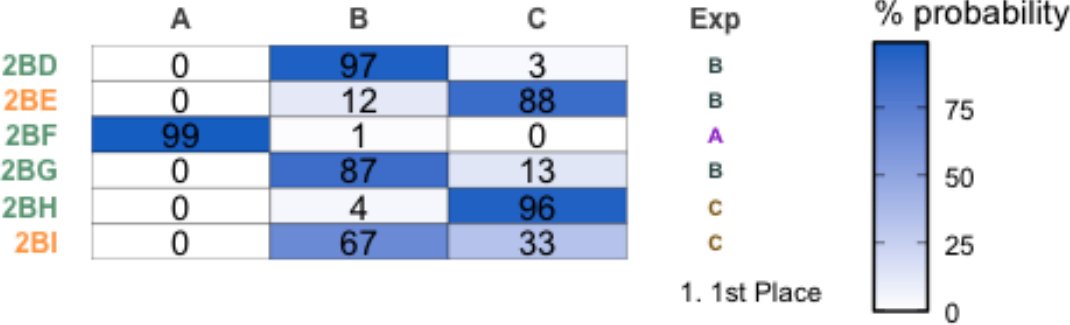
External Validation

Confusion Matrix



External Validation

Probability Heatmap



2nd Place

Table:

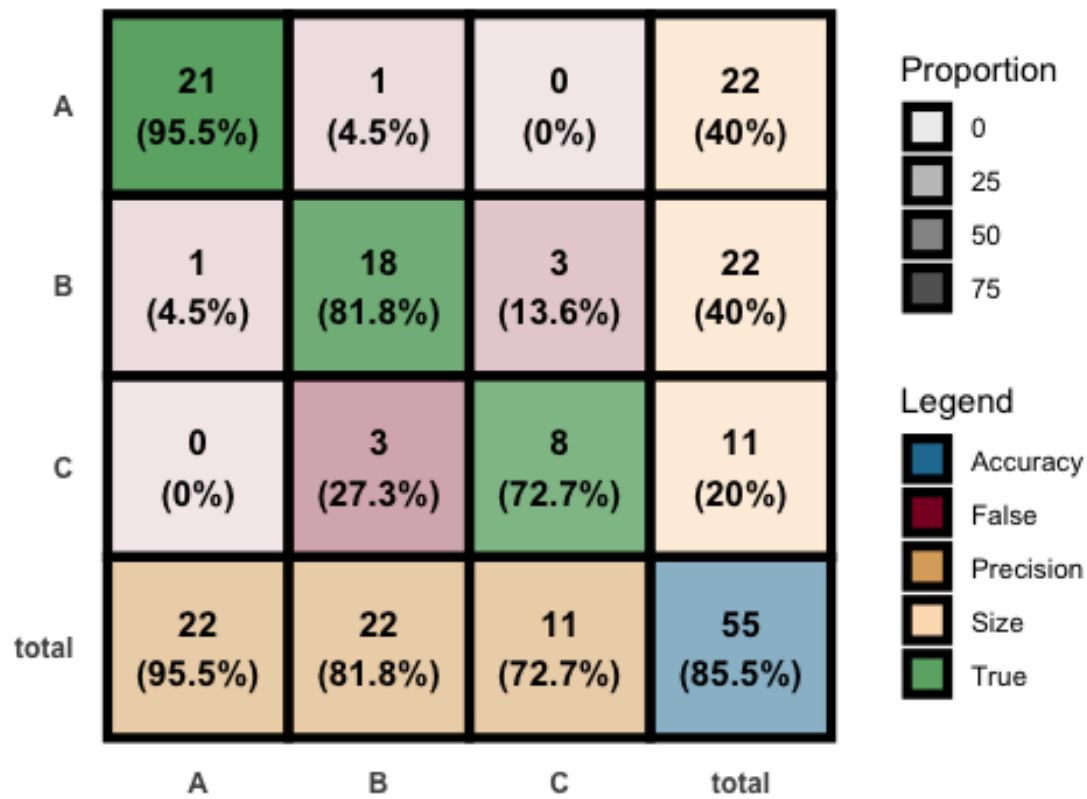
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
85.45%	0.729

Model Coefficients

	(Intercept)	-2-3-	dip_x	dip_y	diff 1 2
2	-260.8328	0.1718610	-9.203331	-14.12606	-157.4286
3	298.0811	-0.1302544	-8.847032	-14.96067	-171.7326

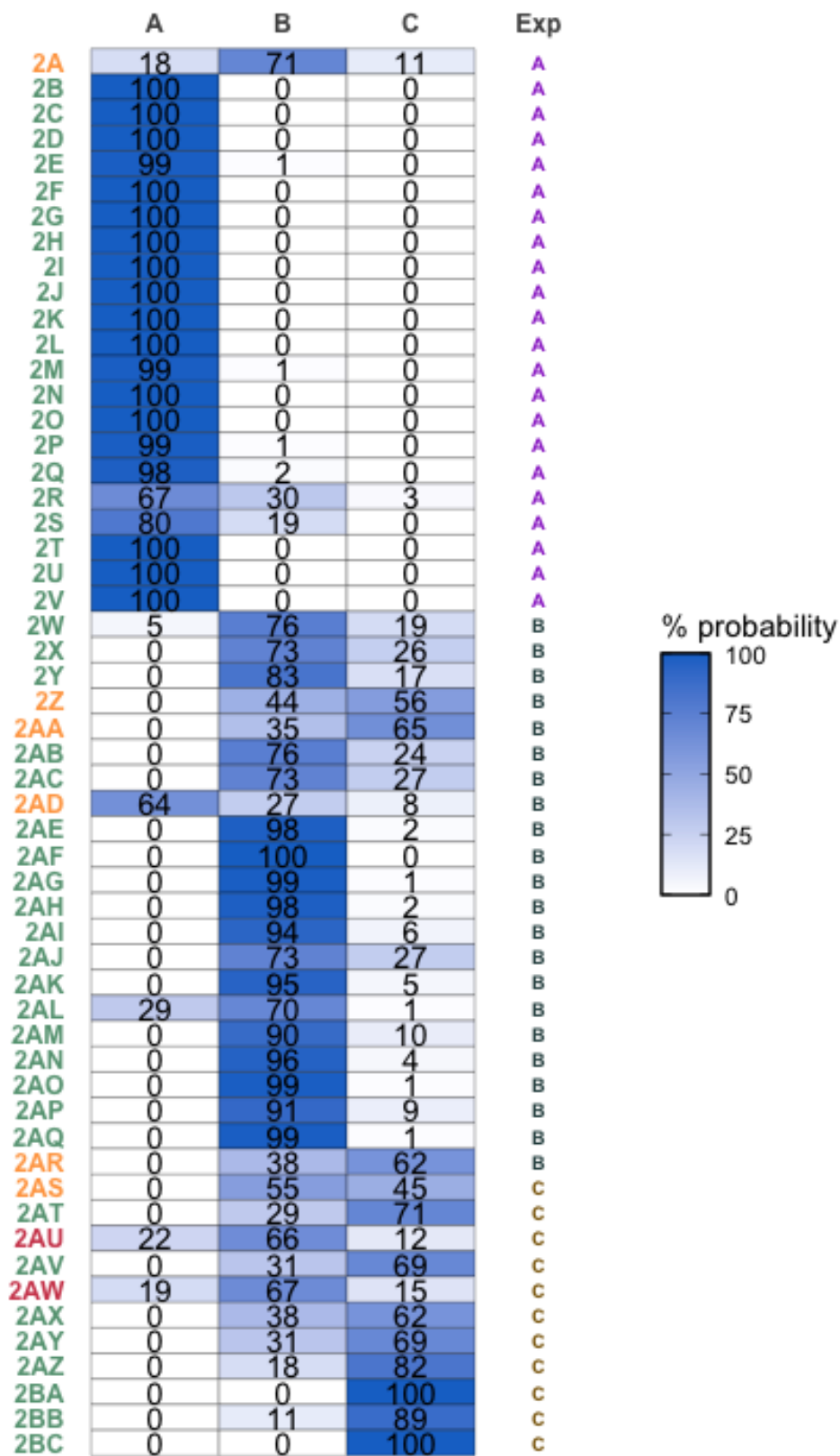
Training Set Confusion Matrix



2. 2nd Place

Training Set

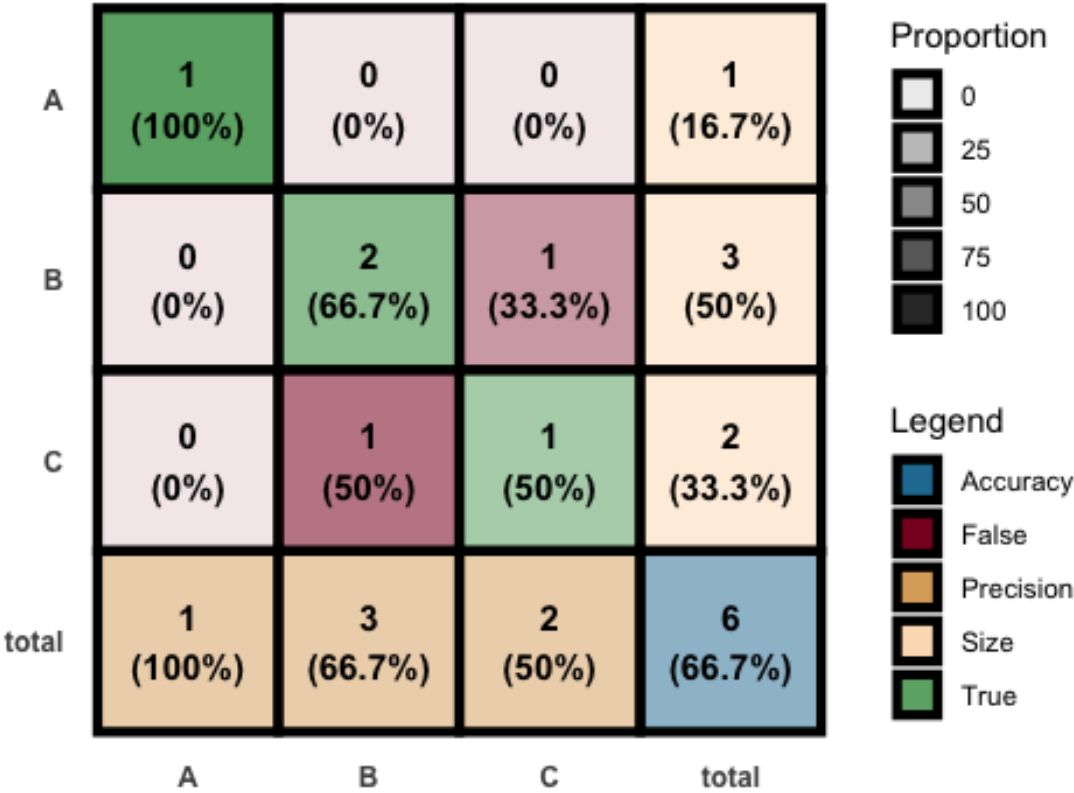
Probability Heatmap



2. 2nd Place

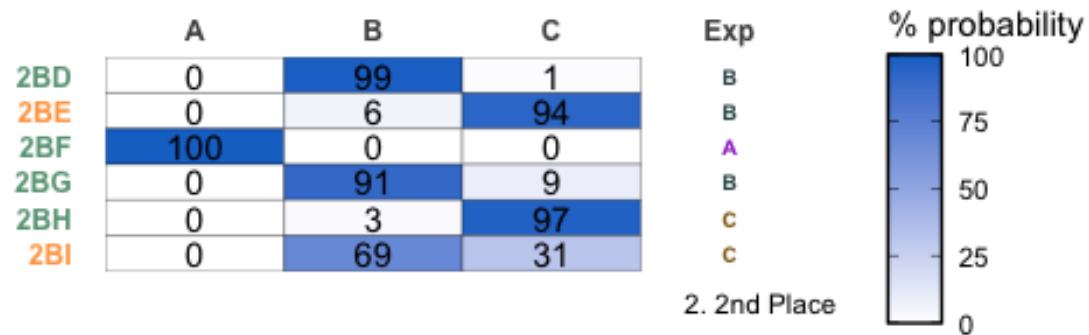
External Validation

Confusion Matrix



External Validation

Probability Heatmap



3rd Place

Table:

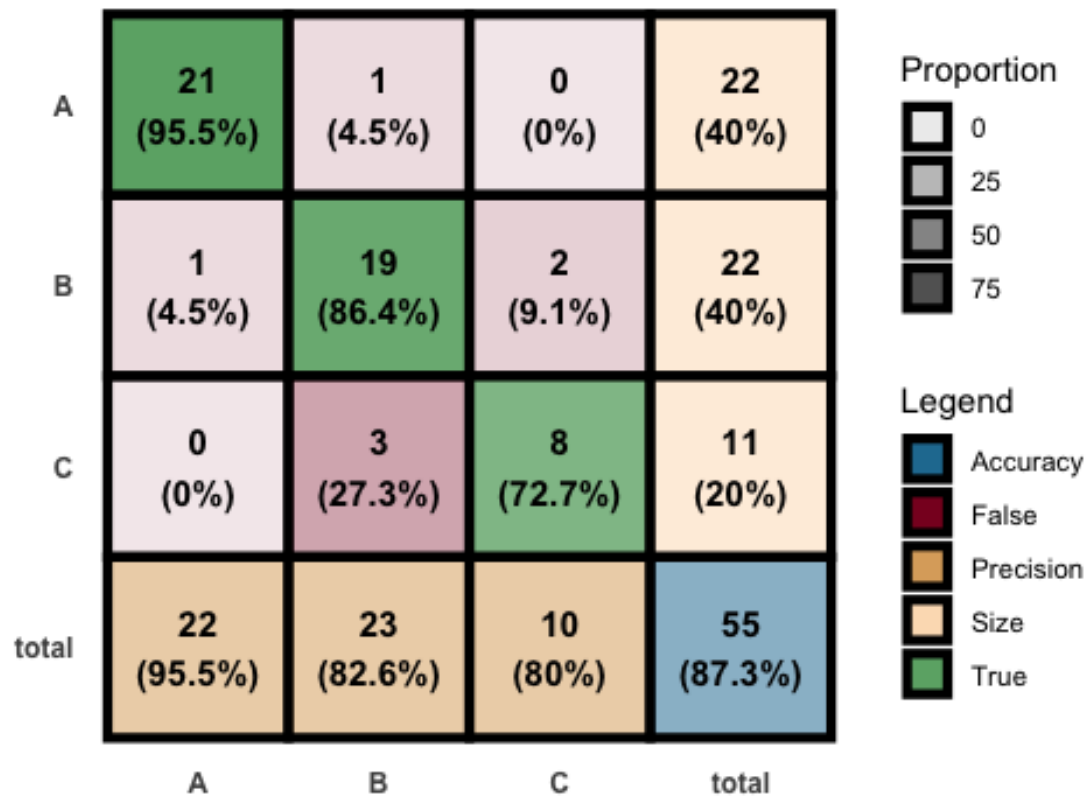
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
87.27%	0.709

Model Coefficients

	(Intercept)	dip_x	dip_y	Dist(2, 3)	NPA_1
2	609.0172	-10.96270	-16.75268	-515.9487	199.5131
3	-641.6359	-10.74353	-17.32803	523.6242	212.4882

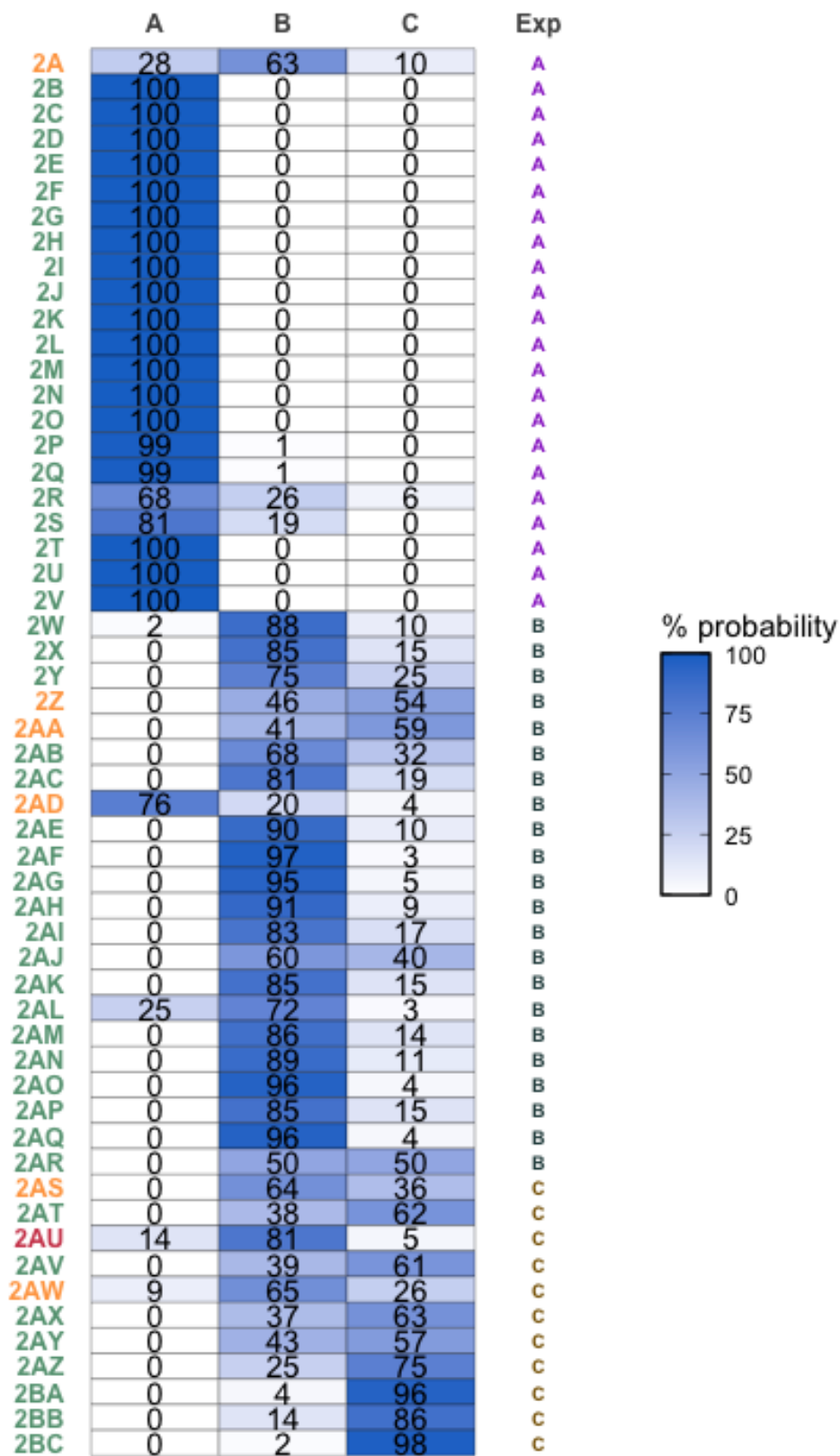
Training Set Confusion Matrix



3. 3rd Place

Training Set

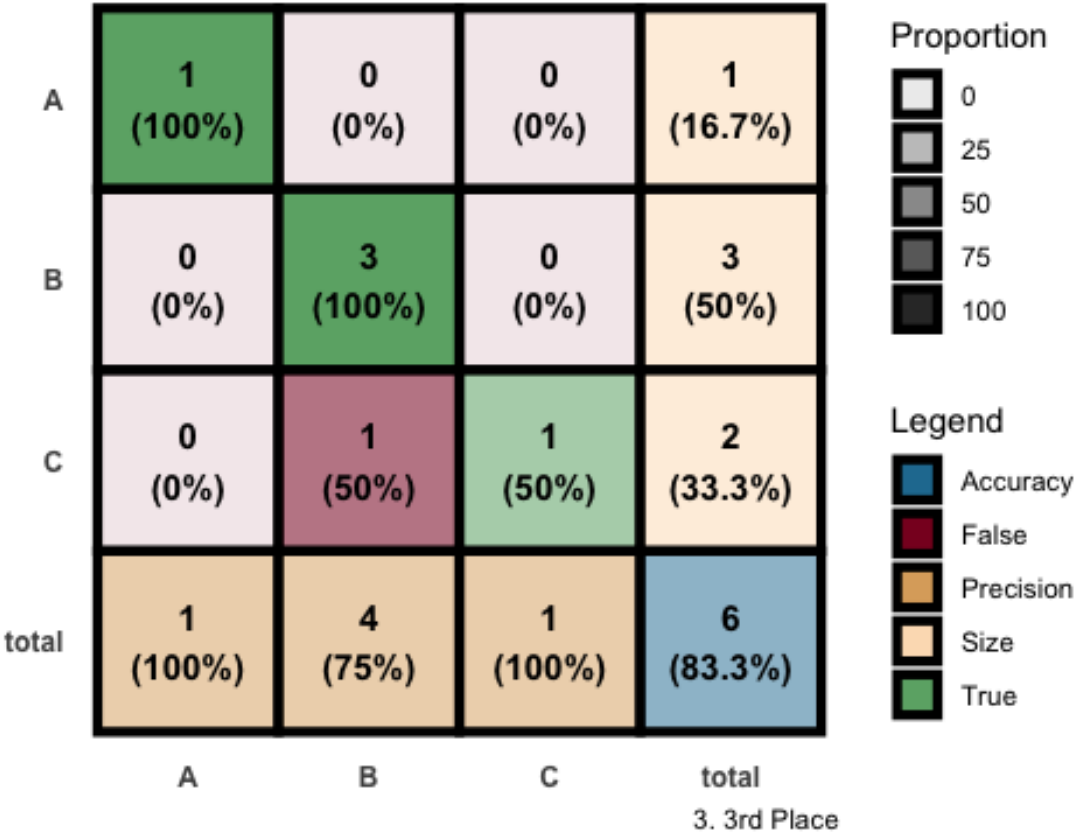
Probability Heatmap



3. 3rd Place

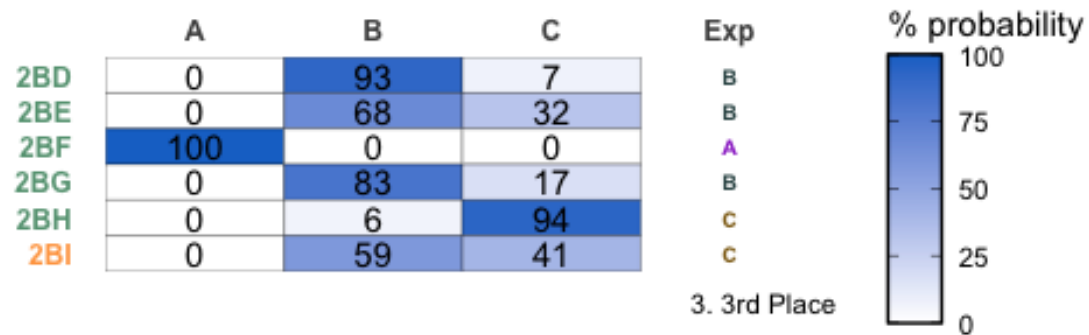
External Validation

Confusion Matrix



External Validation

Probability Heatmap



4th Place

Table:

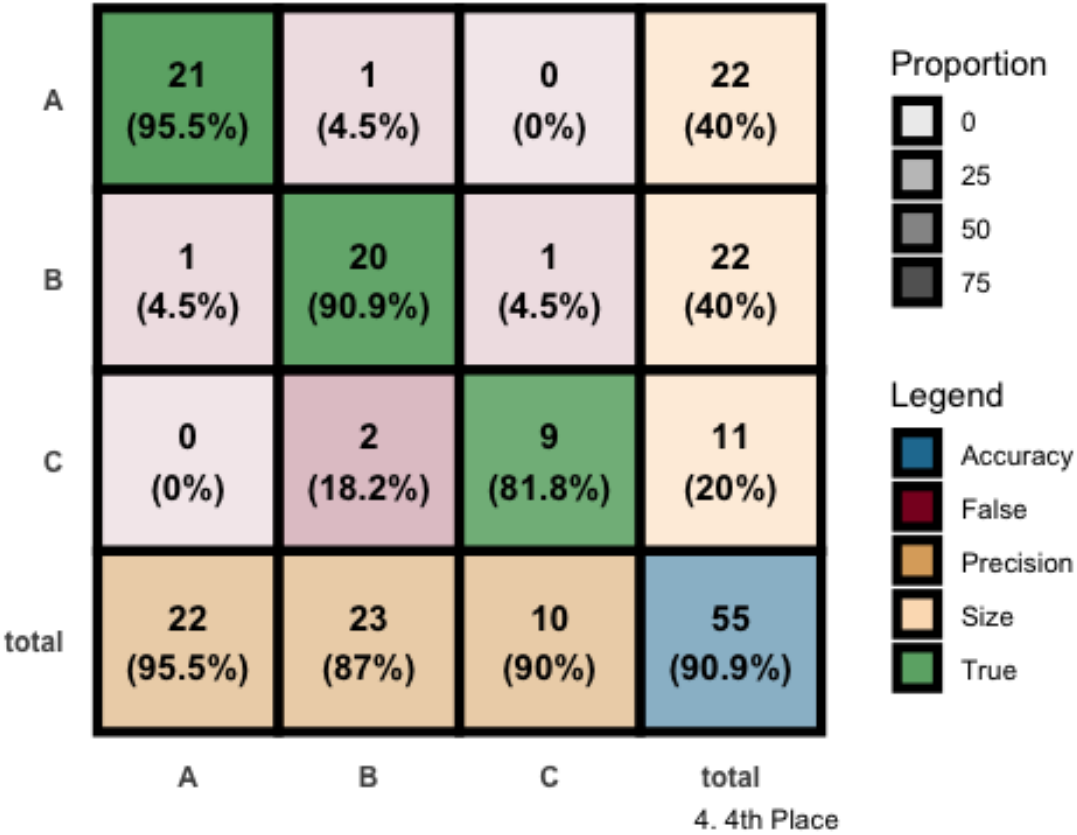
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
90.91%	0.708

Model Coefficients

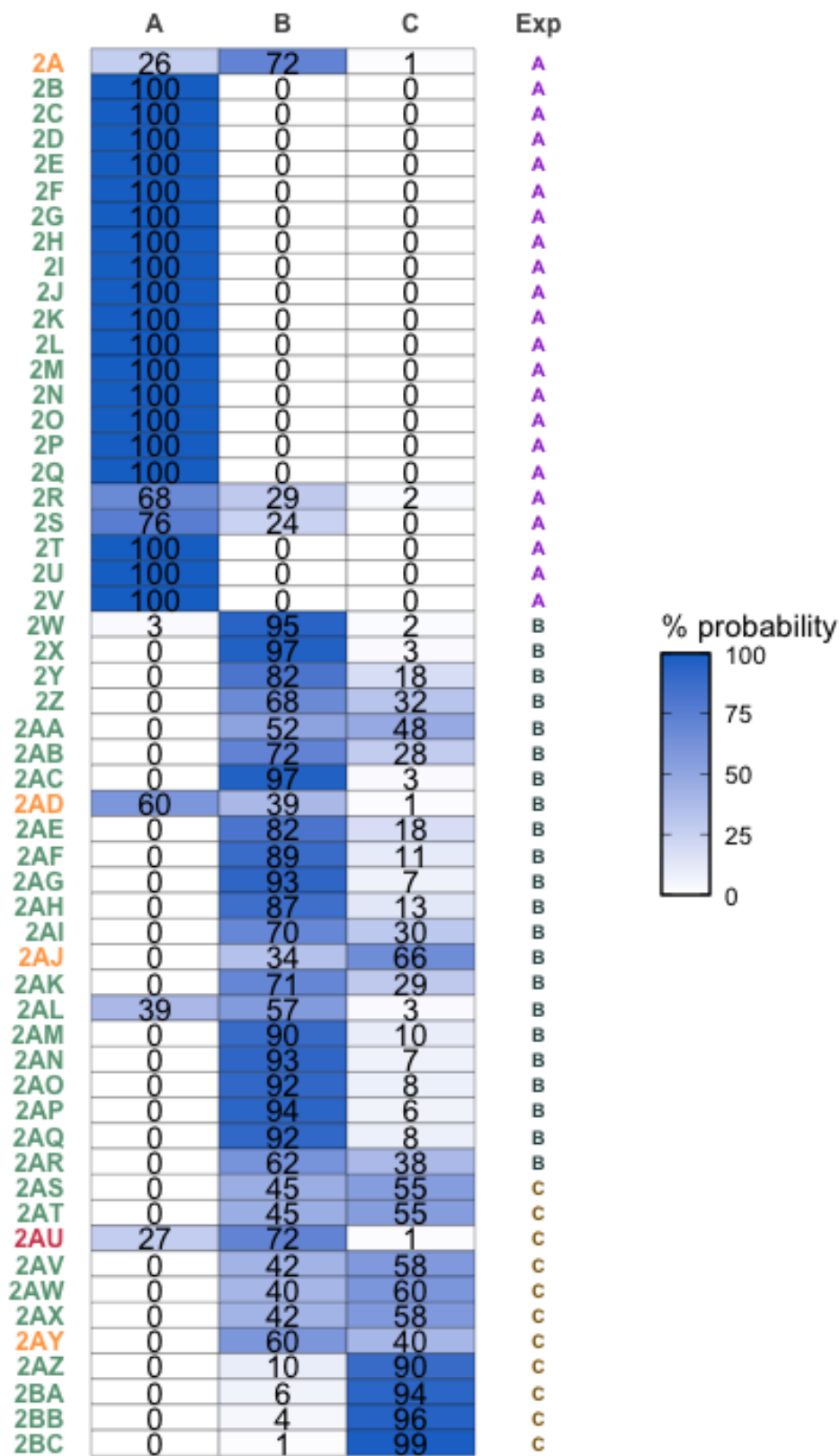
	(Intercept)	dip_x	dip_y	NPA_3	diff 1 2
2	-4.961748	-10.42470	-16.28319	-177.8105	-216.8013
3	-129.526799	-10.42178	-16.34739	-441.1702	-237.4669

Training Set
Confusion Matrix



Training Set

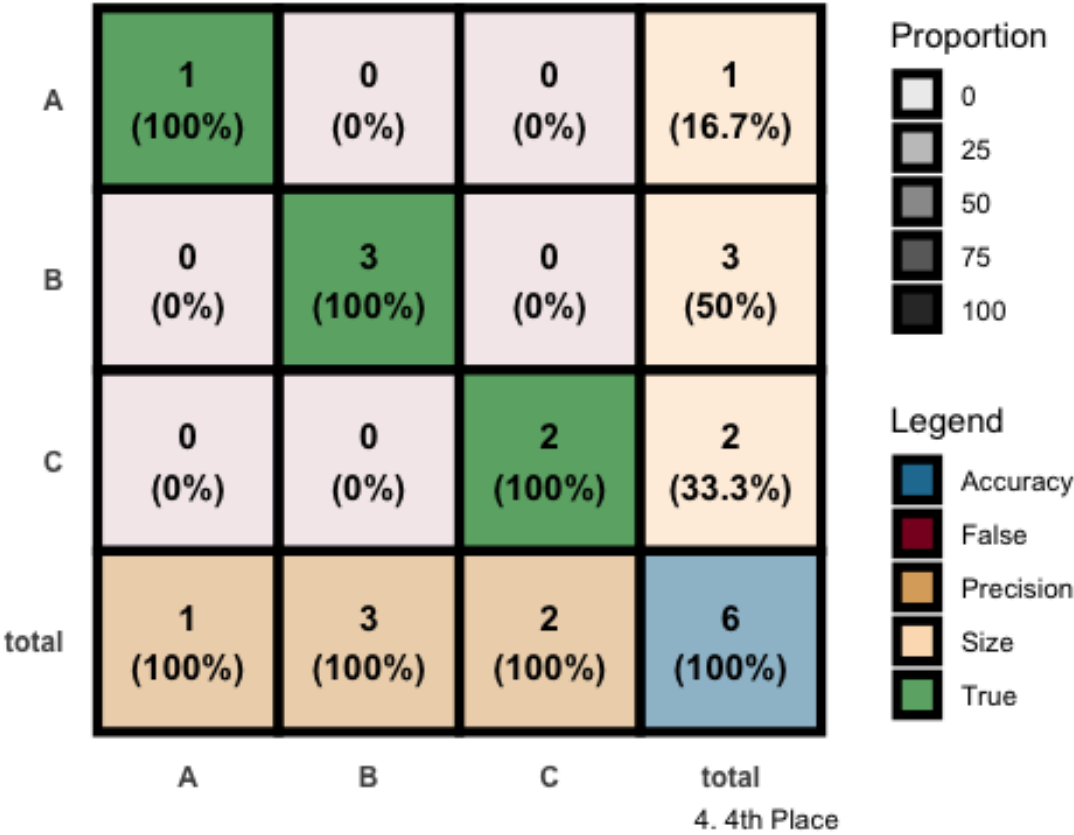
Probability Heatmap



4. 4th Place

External Validation

Confusion Matrix



External Validation

Probability Heatmap

	A	B	C
2BD	0	88	12
2BE	0	86	14
2BF	100	0	0
2BG	0	62	38
2BH	0	2	98
2BI	0	44	56

Exp

B

B

A

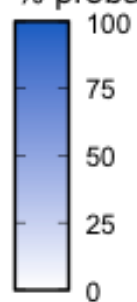
B

C

C

4. 4th Place

% probability



5th Place

Table:

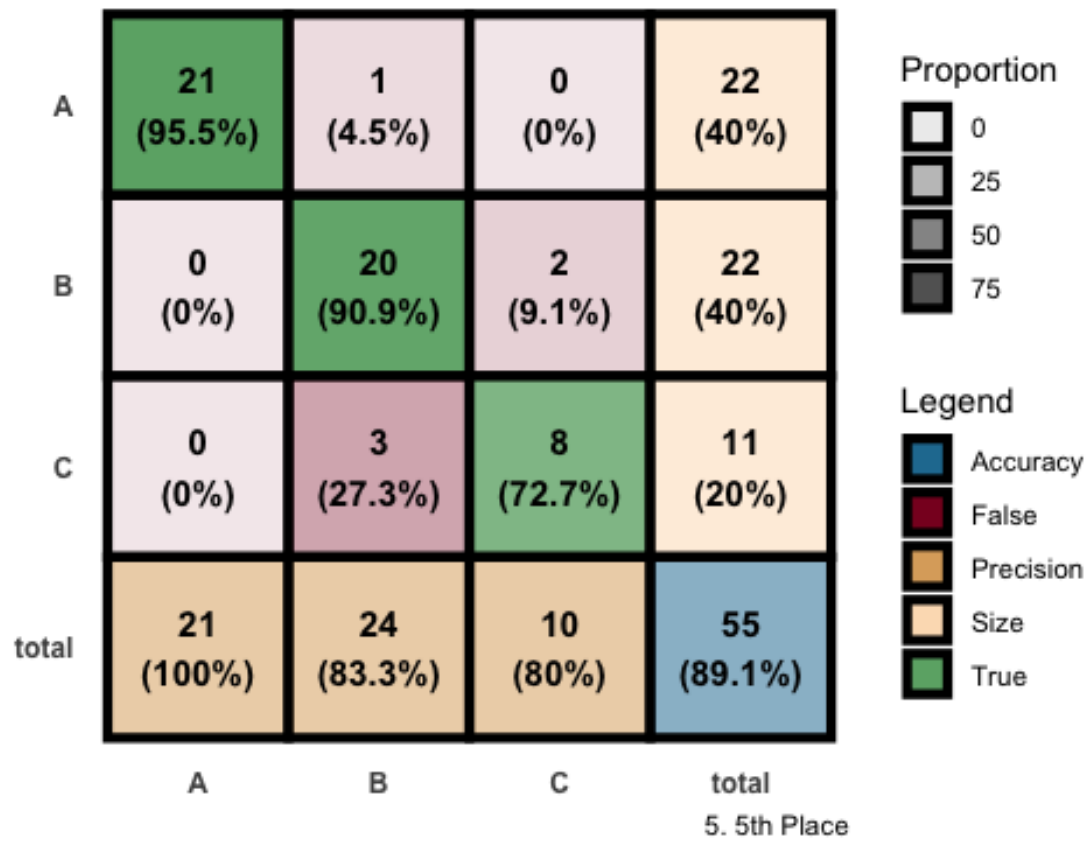
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
89.09%	0.704

Model Coefficients

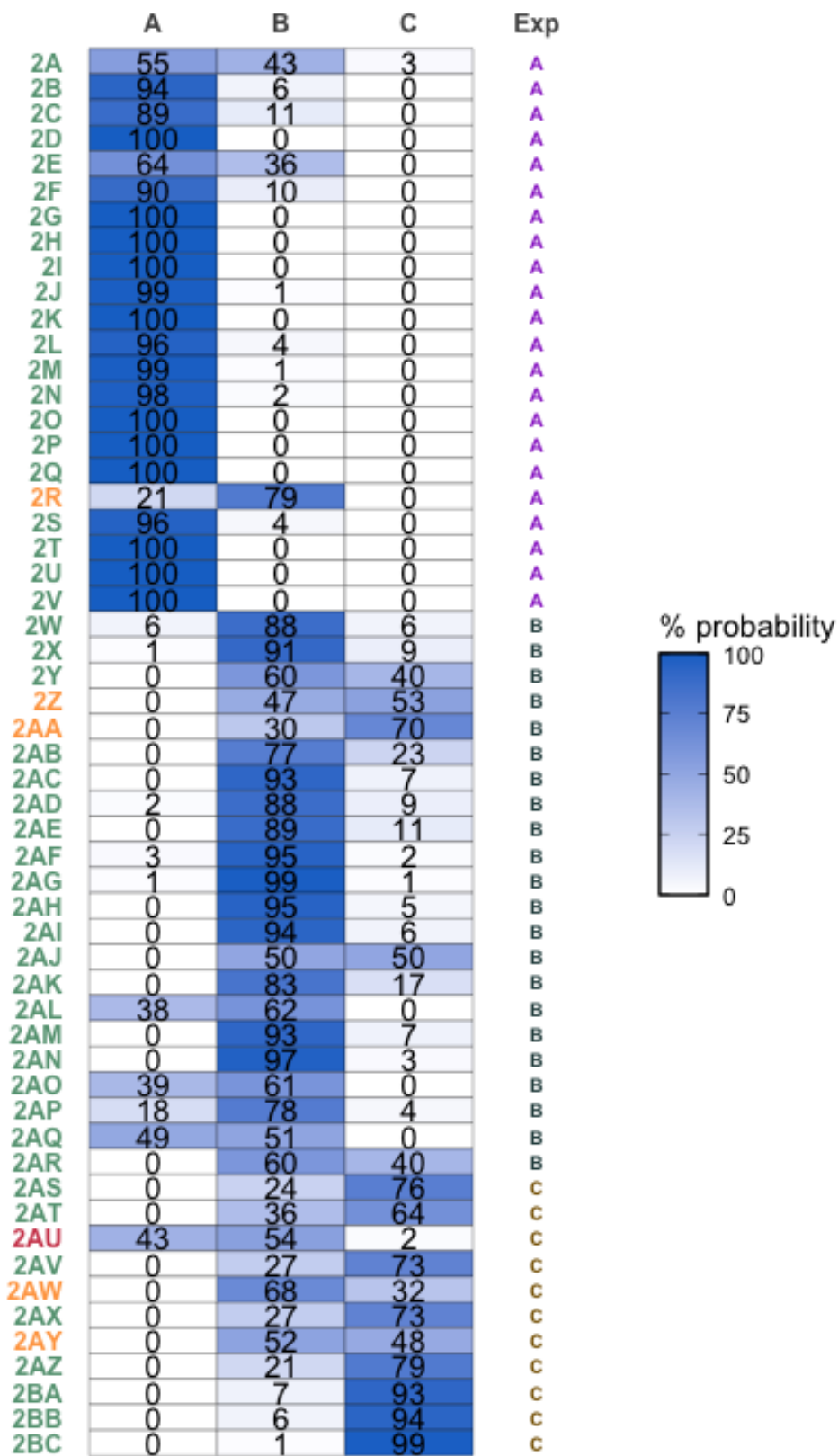
	(Intercept)	dip_y	NPA_3	diff 1 2	loc.B5
2	-269.7012	-4.958572	-698.1891	-150.9582	-1.050146
3	-374.6298	-5.823239	-918.6839	-168.9124	-1.677831

Training Set Confusion Matrix



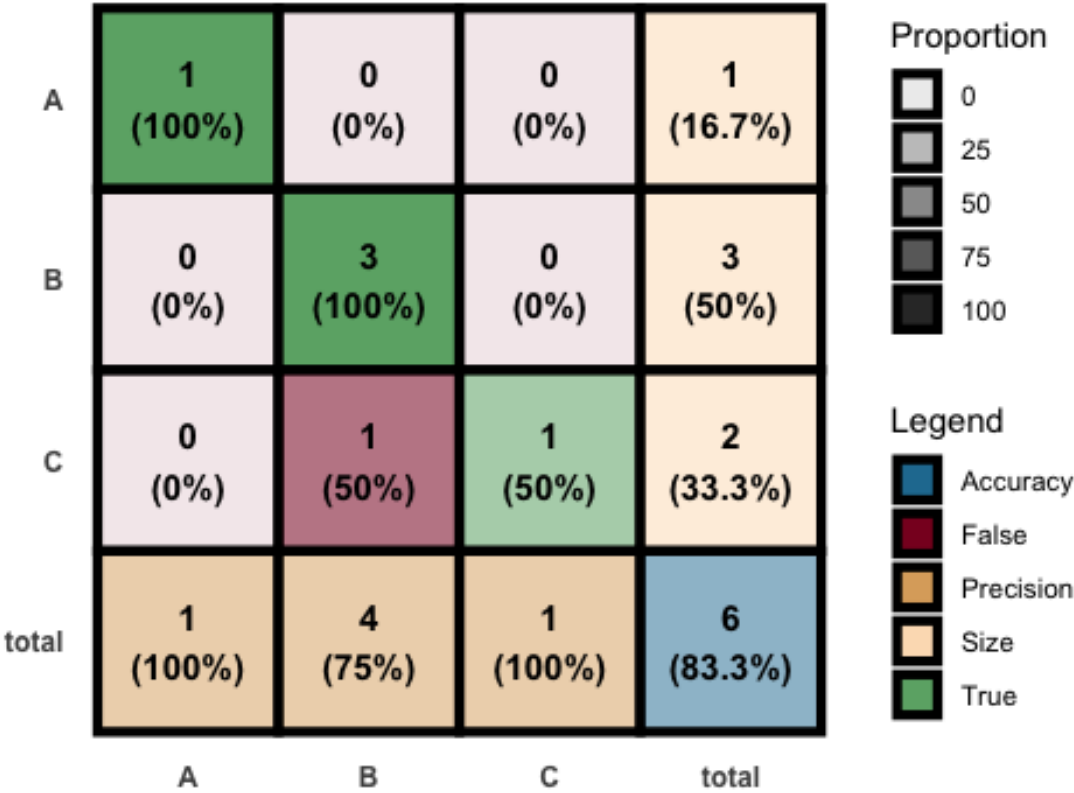
Training Set

Probability Heatmap



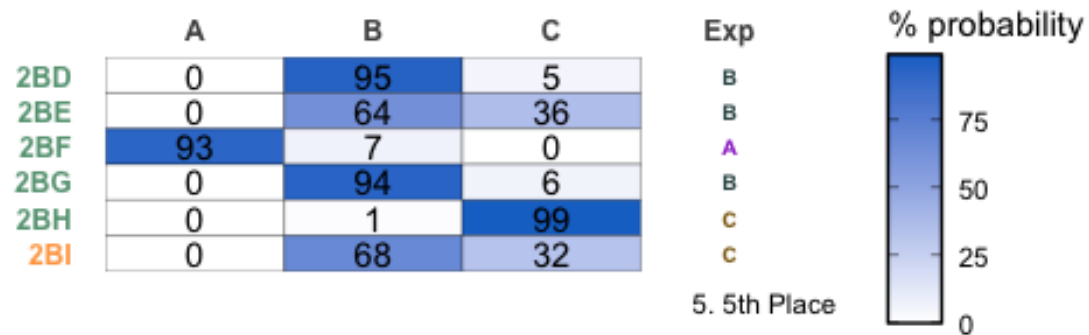
External Validation

Confusion Matrix



External Validation

Probability Heatmap



6th Place

Table:

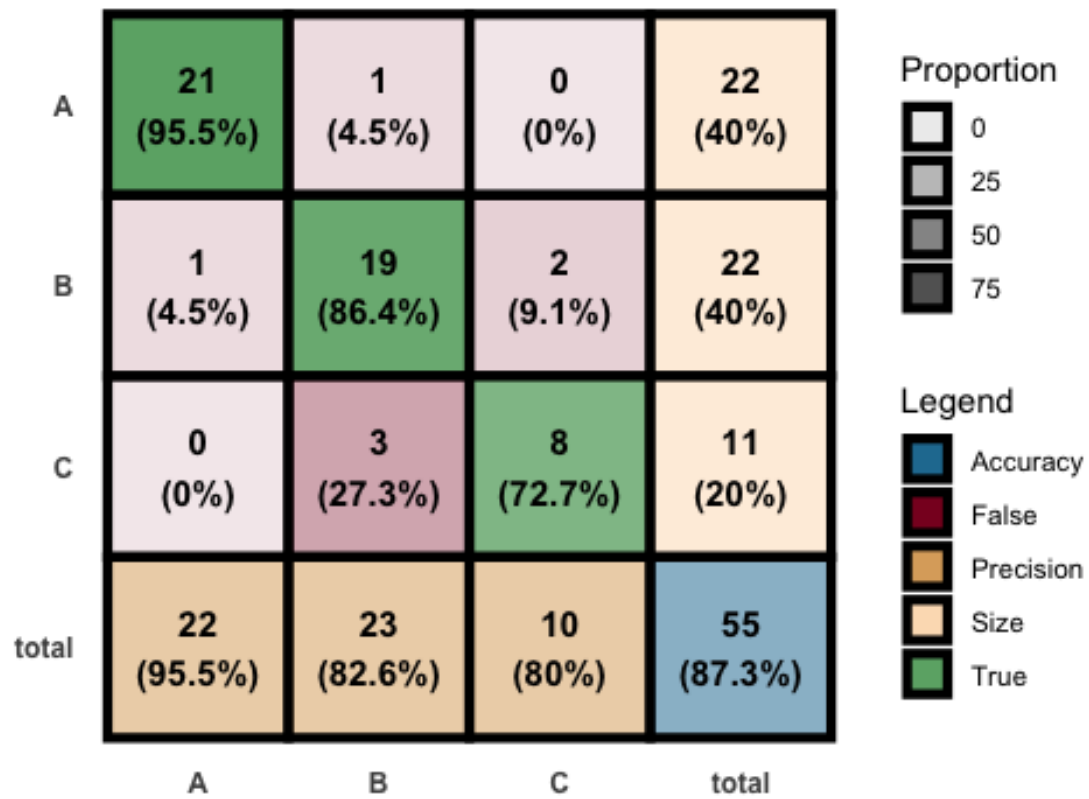
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
87.27%	0.703

Model Coefficients

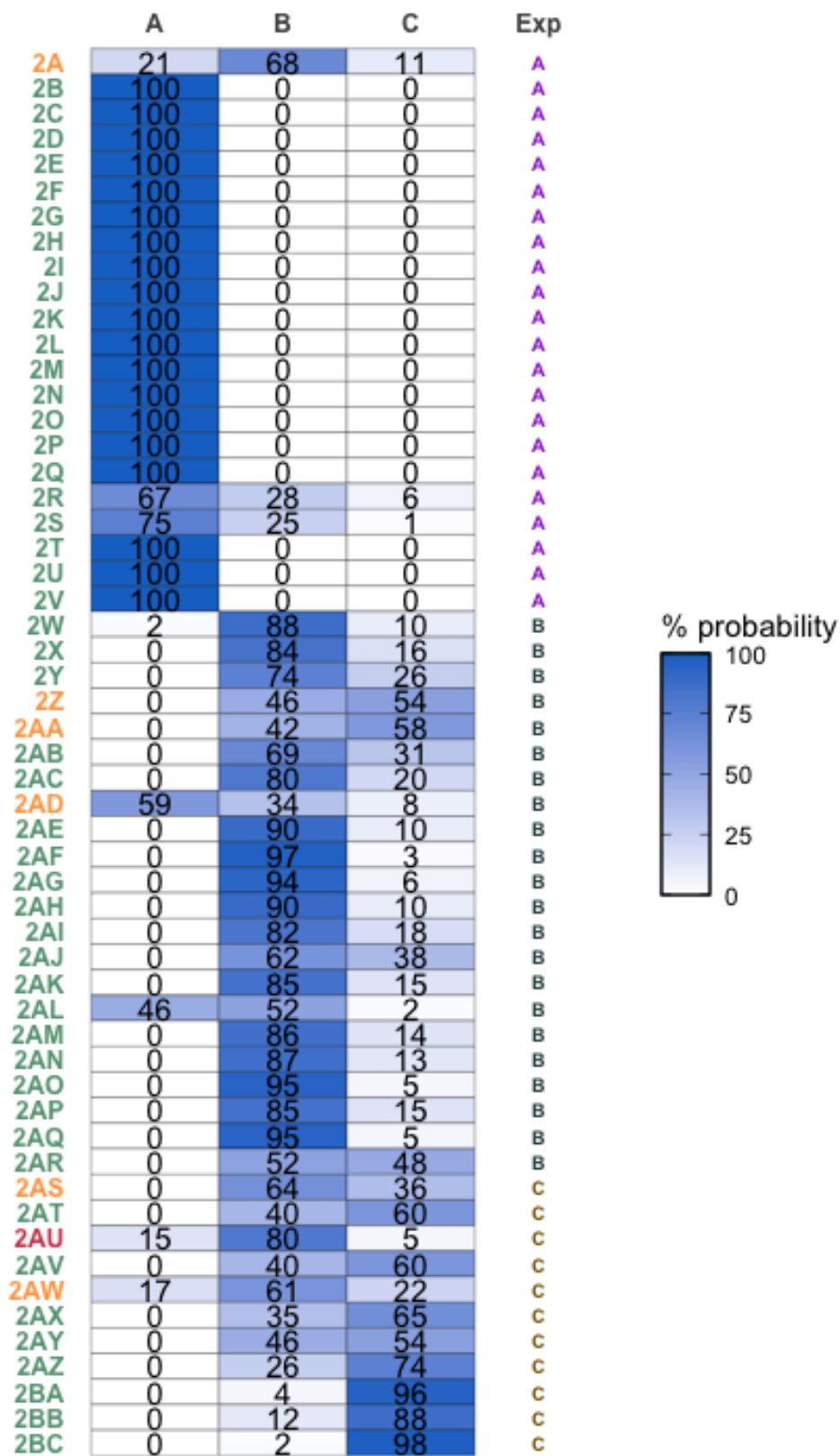
	(Intercept)	dip_x	dip_y	Dist(2, 3)	diff 1 2
2	592.4418	-10.22089	-16.17417	-432.5536	-195.7916
3	-527.3451	-10.06336	-16.80914	502.2552	-208.2112

Training Set Confusion Matrix



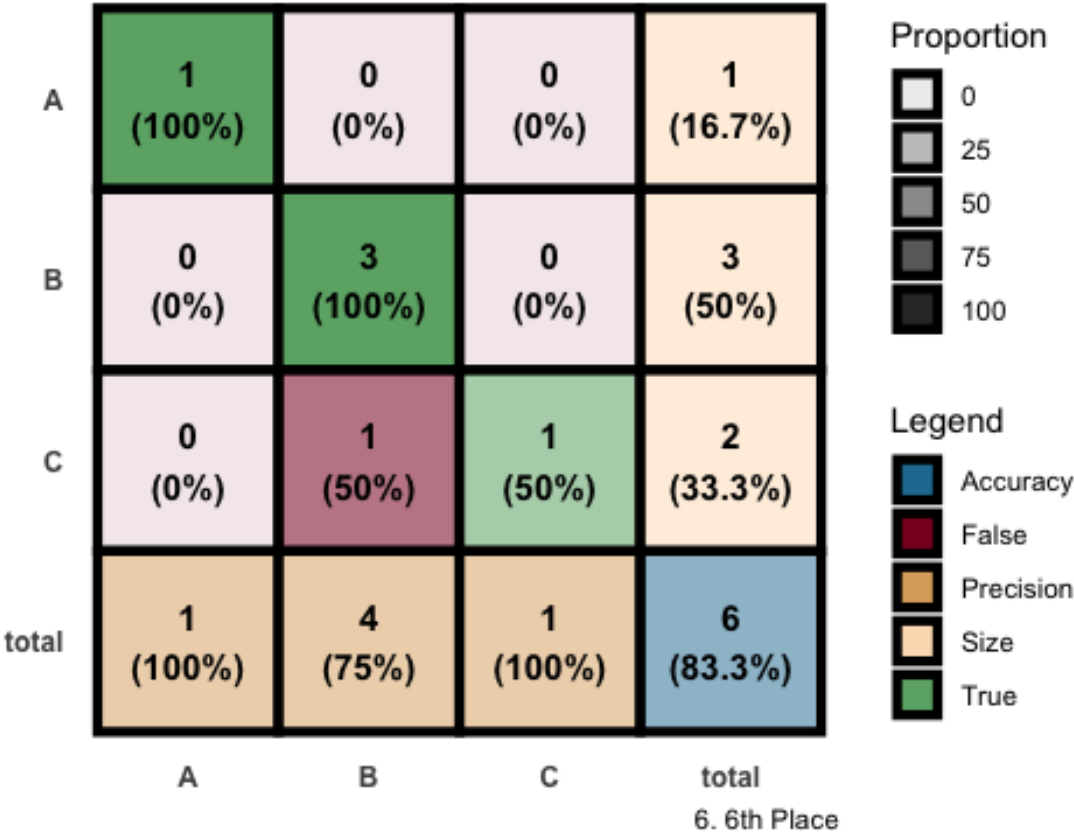
Training Set

Probability Heatmap



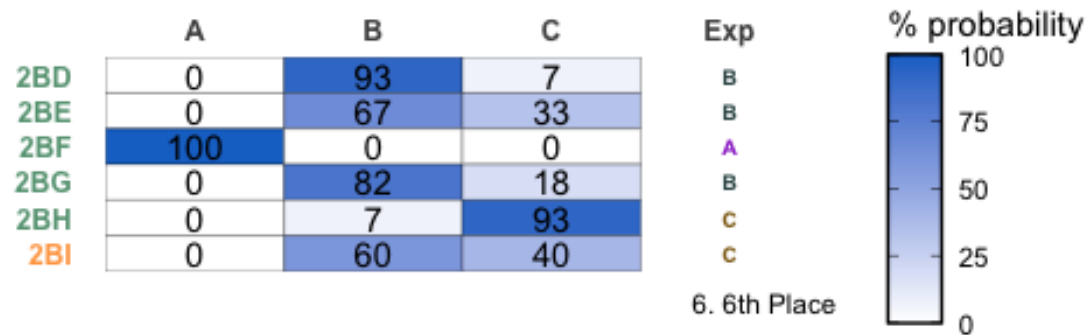
External Validation

Confusion Matrix



External Validation

Probability Heatmap



7th Place

Table:

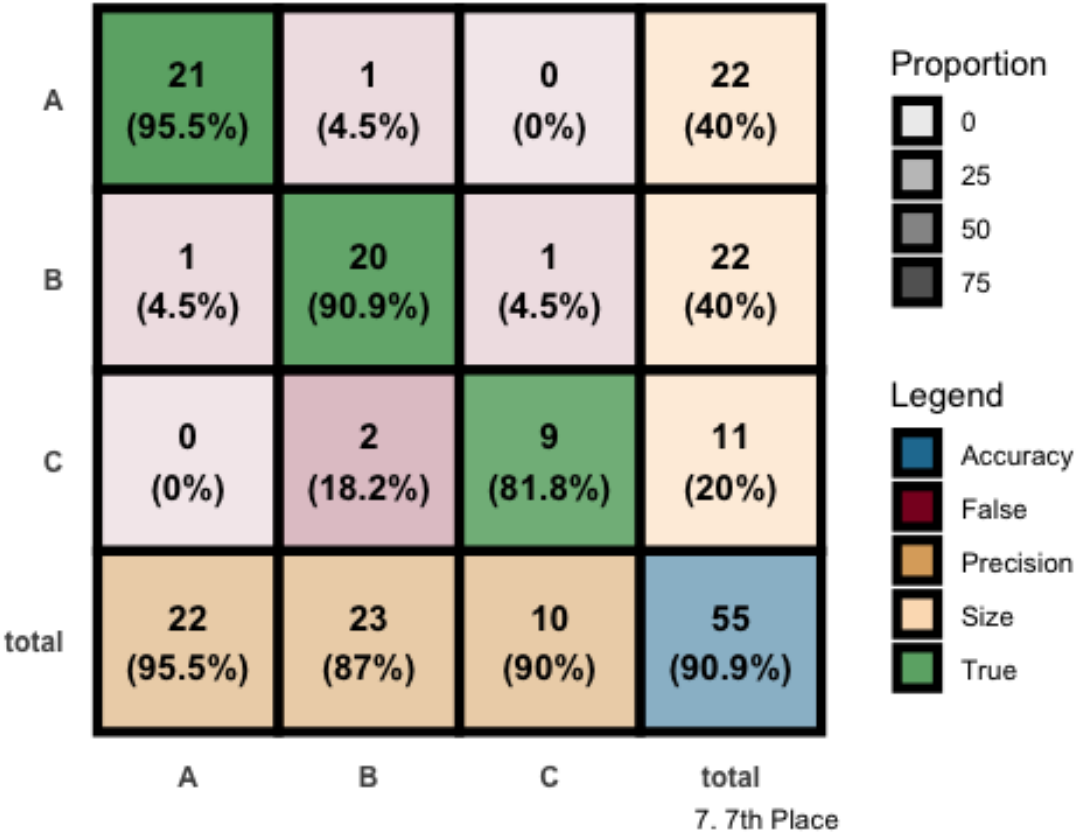
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
90.91%	0.702

Model Coefficients

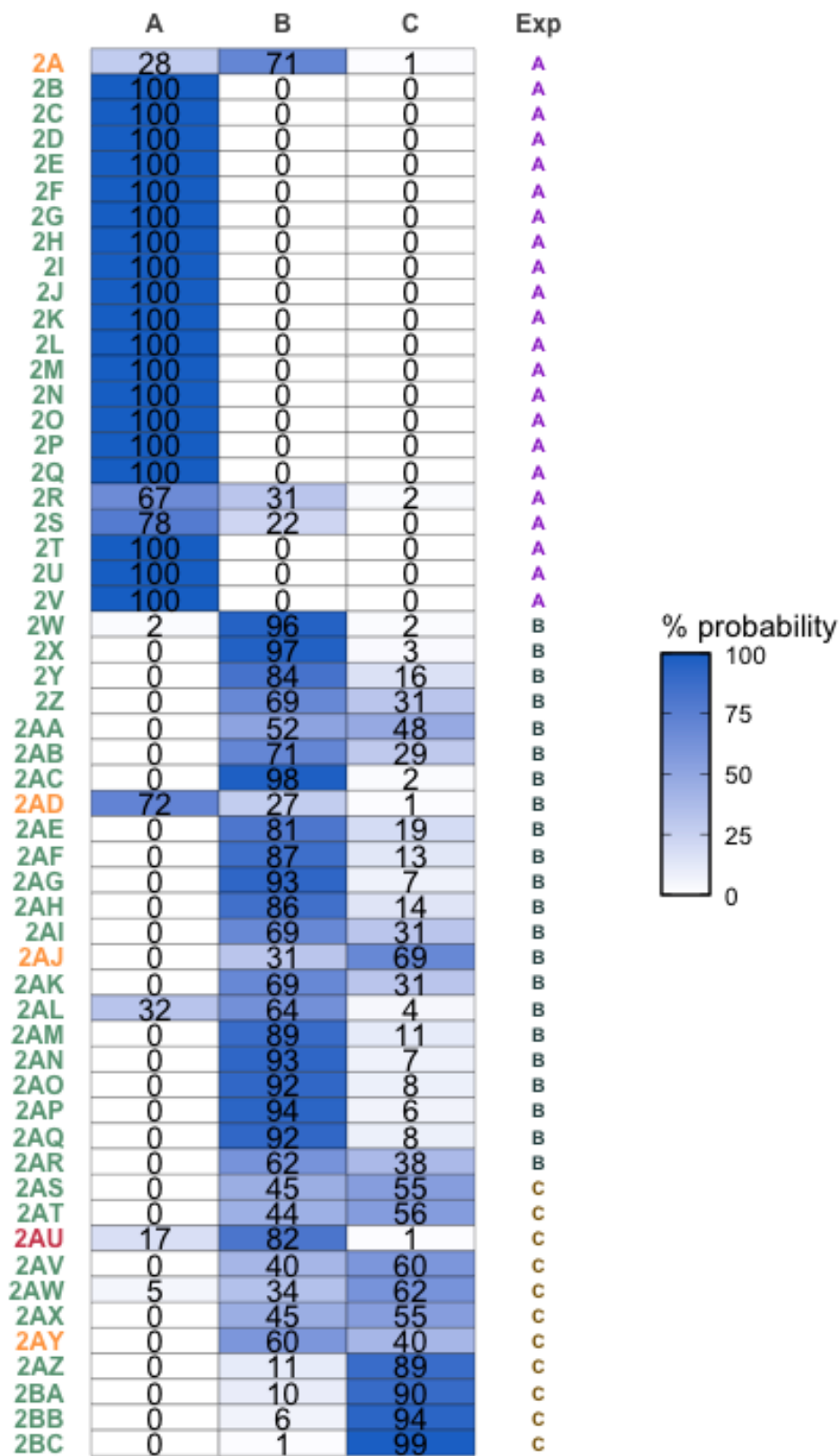
	(Intercept)	dip_x	dip_y	NPA_1	NPA_3
2	12.21291	-10.86157	-16.91666	206.4310	43.86709
3	-127.12032	-10.85380	-16.84775	226.9644	-232.03913

Training Set
Confusion Matrix



Training Set

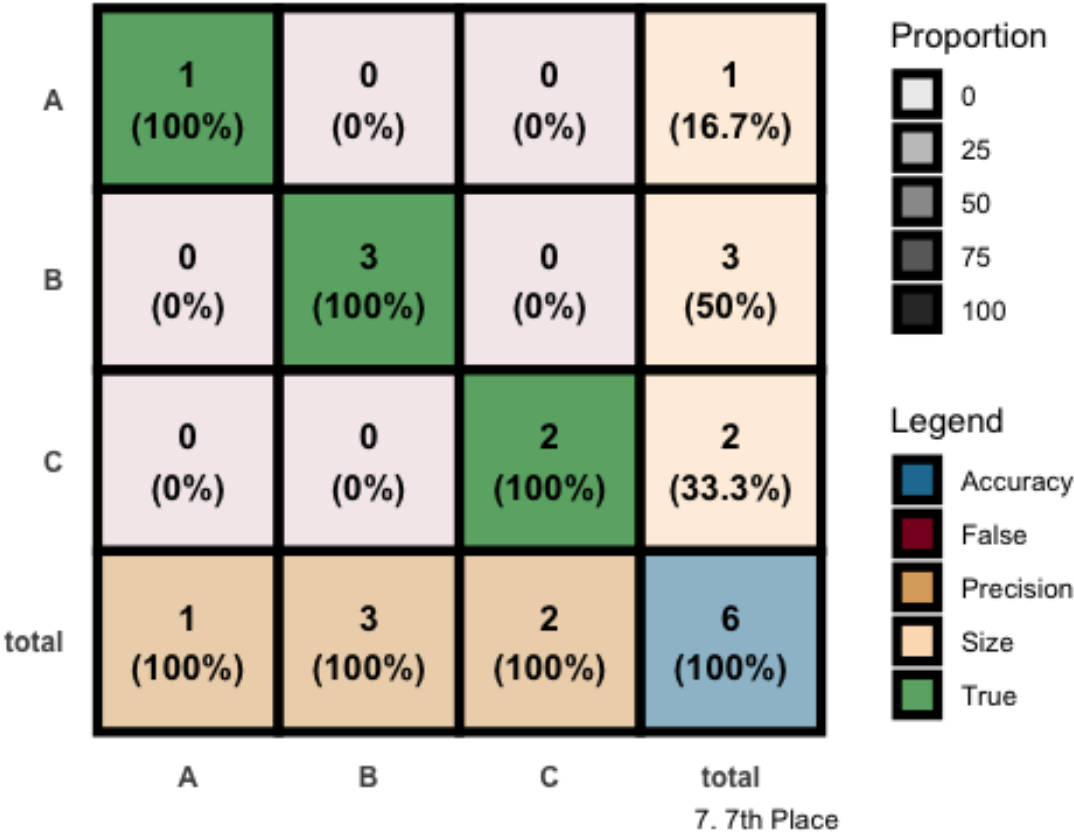
Probability Heatmap



7. 7th Place

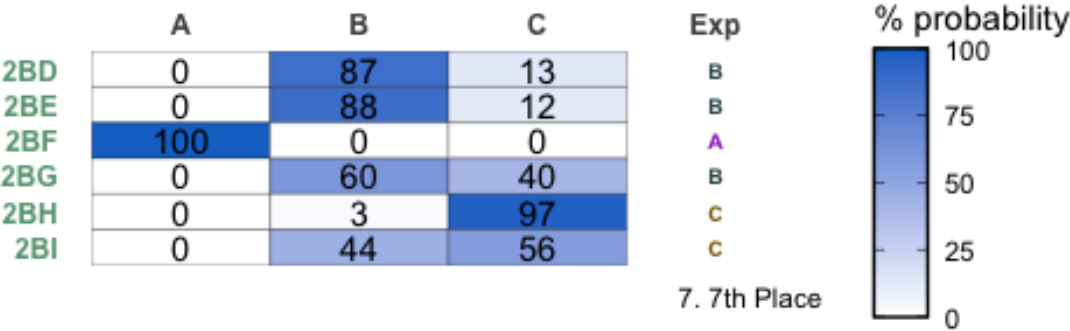
External Validation

Confusion Matrix



External Validation

Probability Heatmap



8th Place

Table:

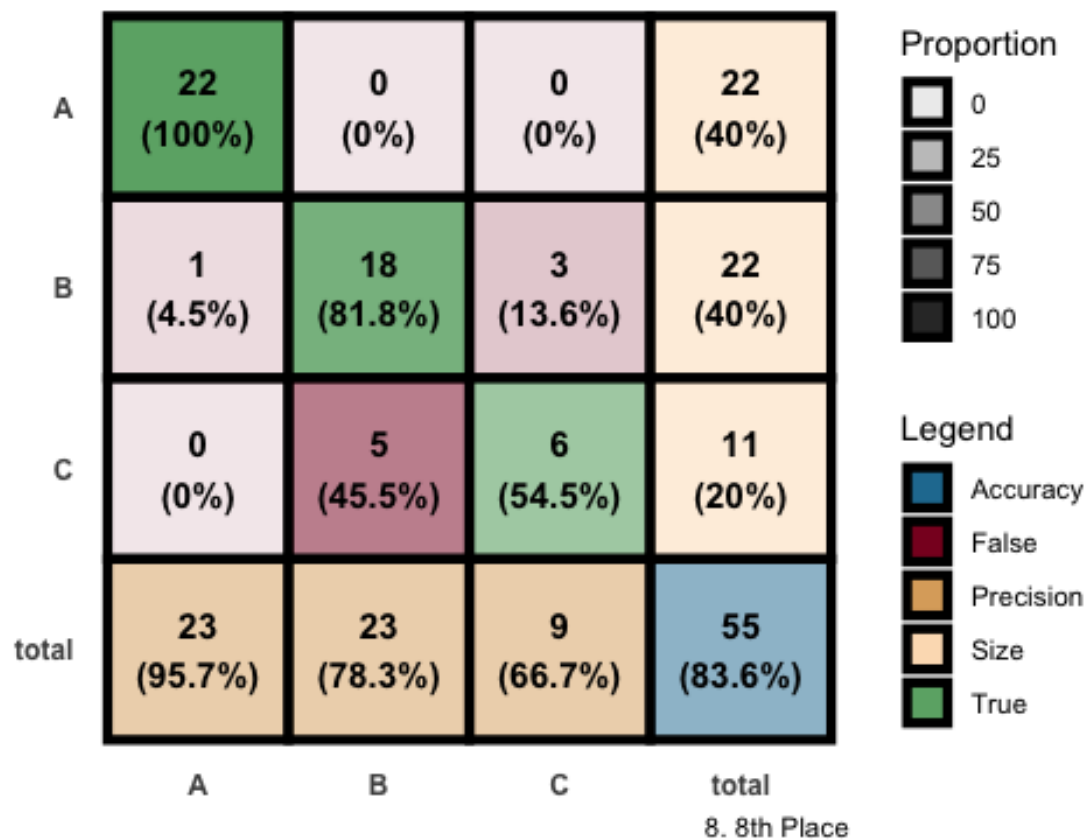
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
83.64%	0.693

Model Coefficients

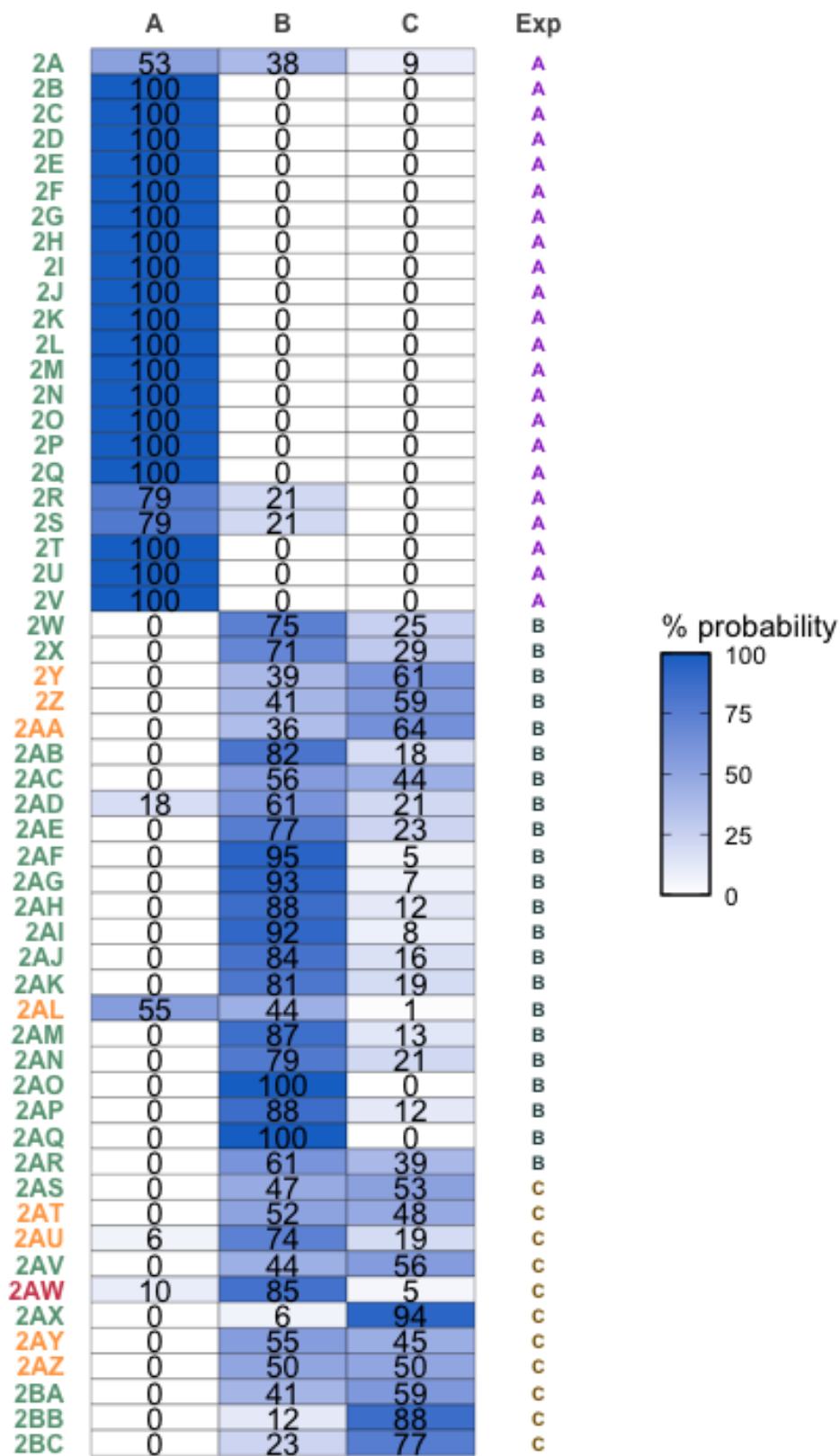
	(Intercept)	dip_x	dip_y	NPA_1	loc.B5
2	3.4312408	-12.64828	-24.39738	362.6605	-0.9819199
3	0.9534051	-13.08195	-26.21570	379.6056	-1.6053849

Training Set Confusion Matrix



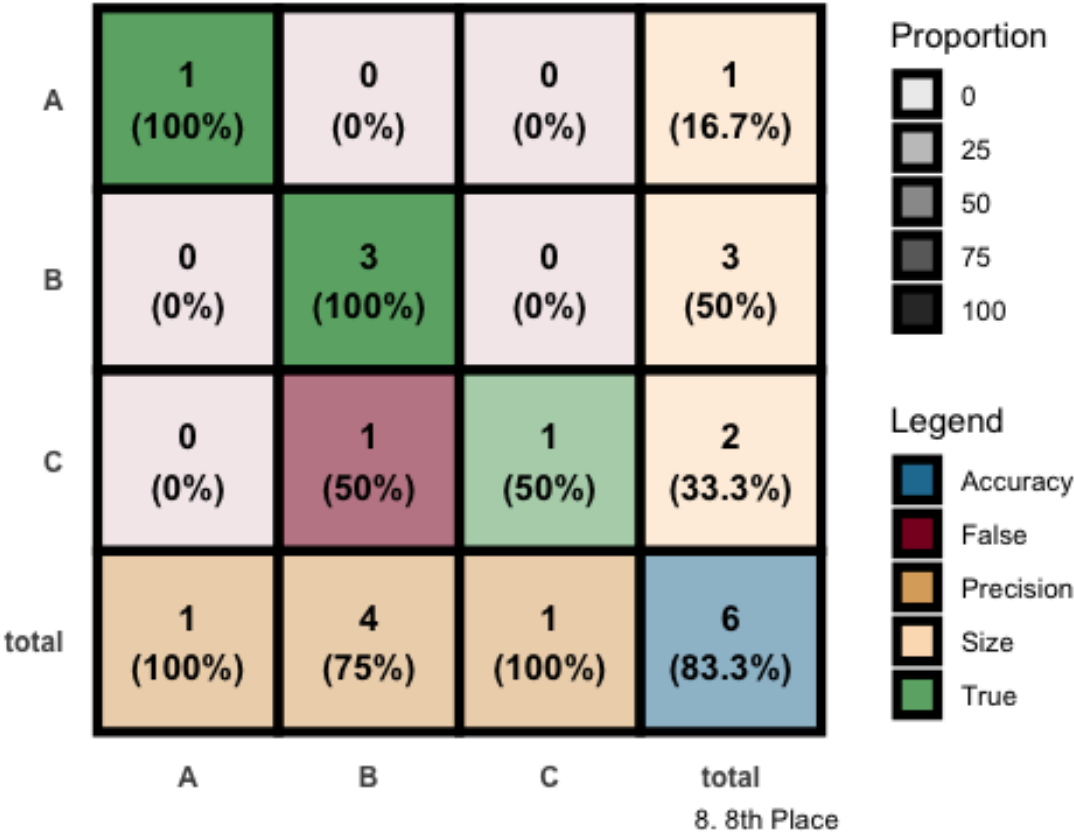
Training Set

Probability Heatmap



External Validation

Confusion Matrix



External Validation

Probability Heatmap

	A	B	C
2BD	0	91	9
2BE	0	58	42
2BF	100	0	0
2BG	0	92	8
2BH	0	7	93
2BI	0	73	27

Exp

B

B

A

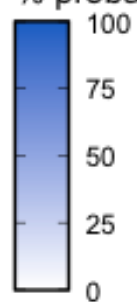
B

C

C

8. 8th Place

% probability



9th Place

Table:

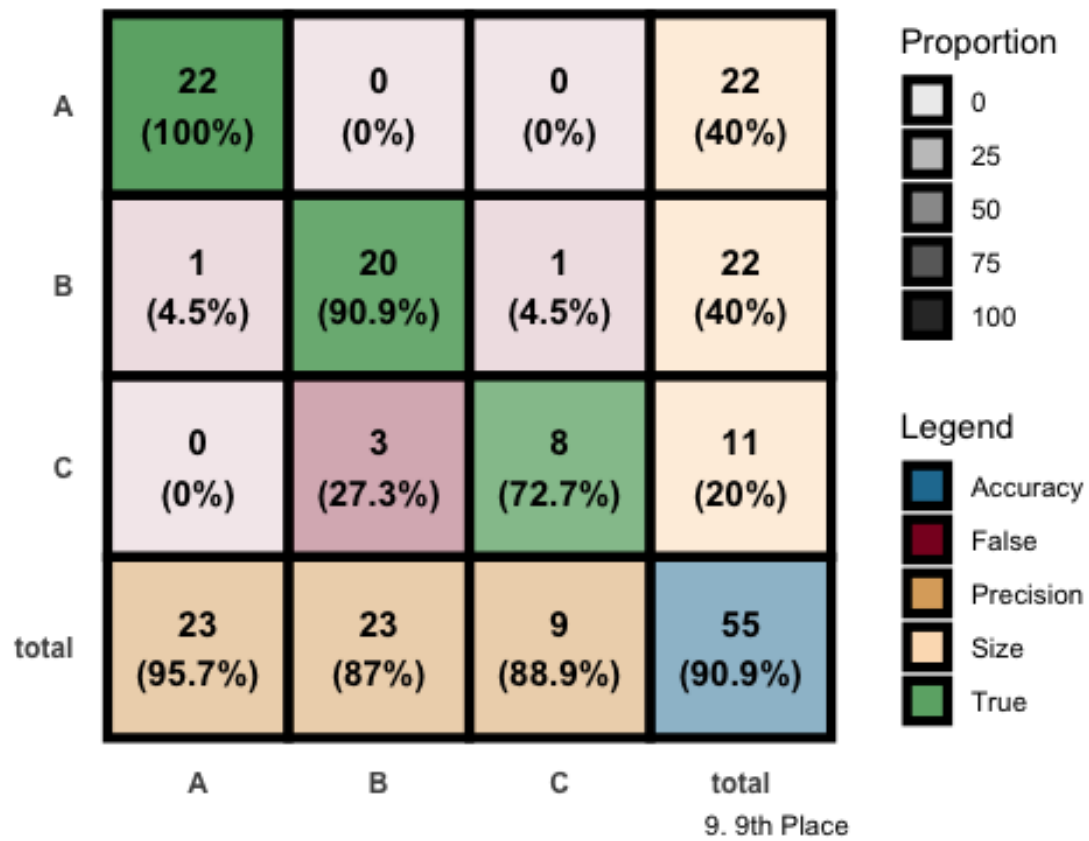
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
90.91%	0.69

Model Coefficients

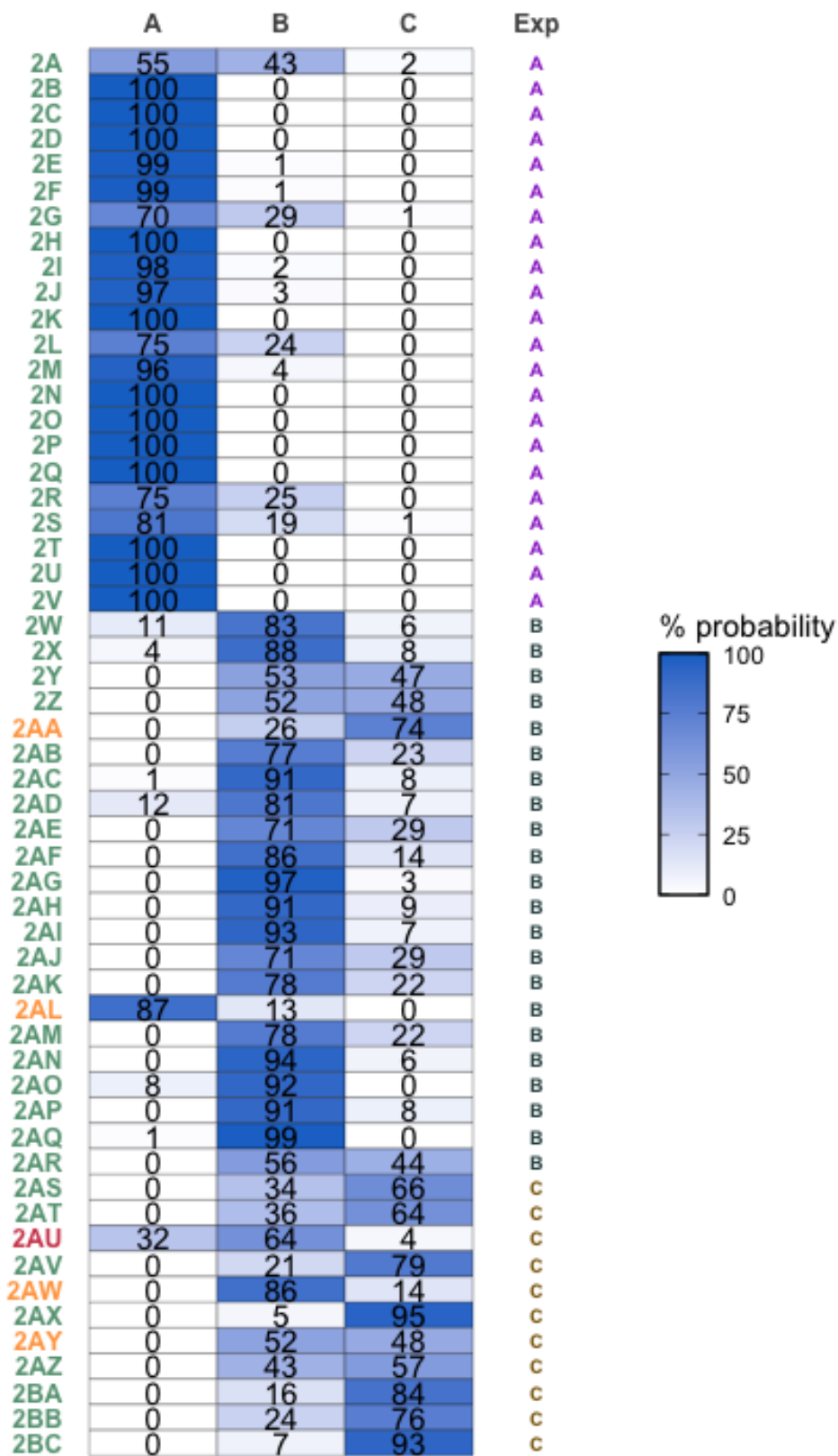
	(Intercept)	Total	NPA_1	diff 2 3	loc.B5
2	-580.6574	7.095702	115.3785	634.3484	-2.060305
3	-702.7903	8.362575	139.5112	765.8227	-2.841061

Training Set Confusion Matrix

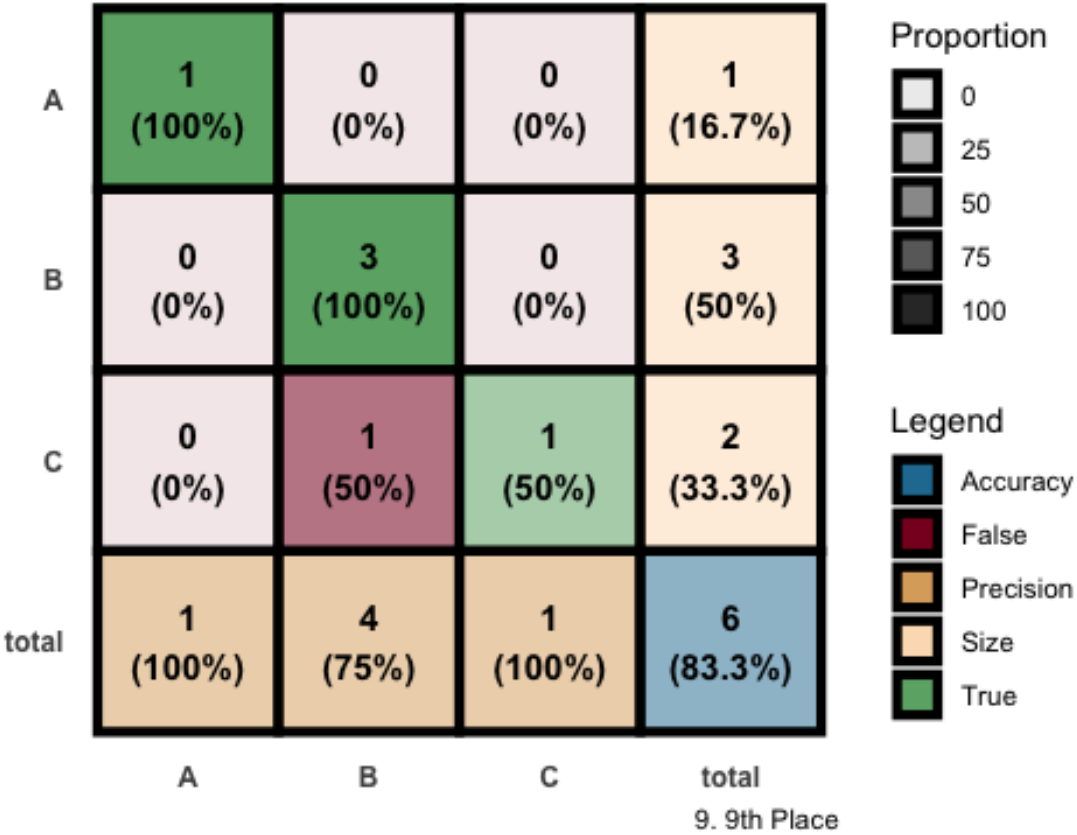


Training Set

Probability Heatmap

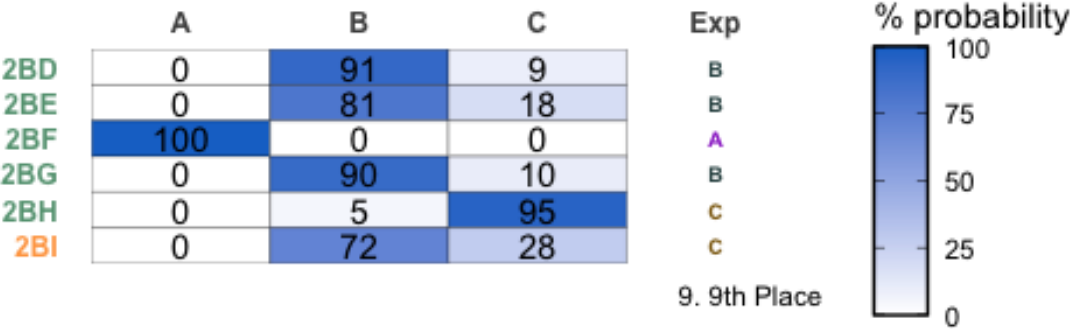


External Validation
Confusion Matrix



External Validation

Probability Heatmap



10th Place

Table:

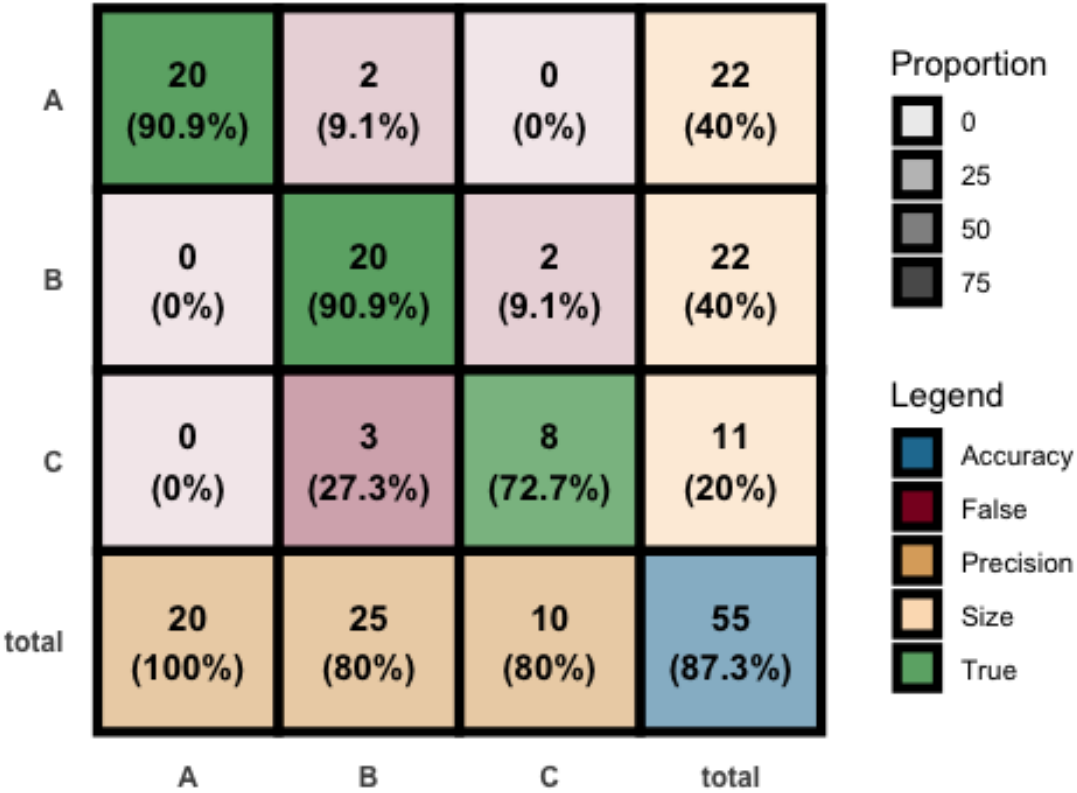
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
87.27%	0.689

Model Coefficients

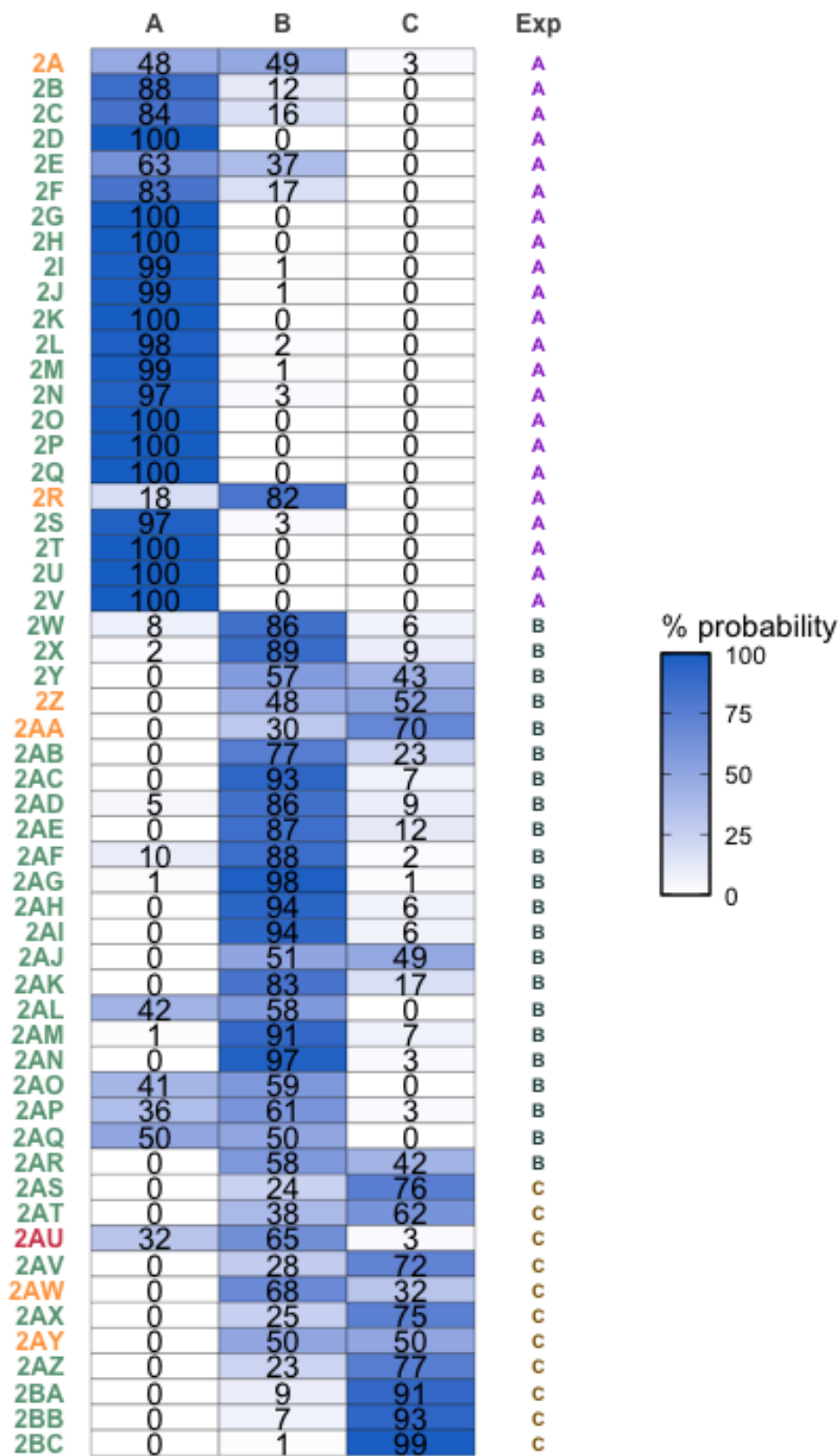
	(Intercept)	dip_y	NPA_1	NPA_3	loc.B5
2	-193.2967	-4.466947	109.8627	-407.1690	-0.8615639
3	-303.4575	-5.338075	128.9827	-623.7929	-1.5249576

Training Set
Confusion Matrix



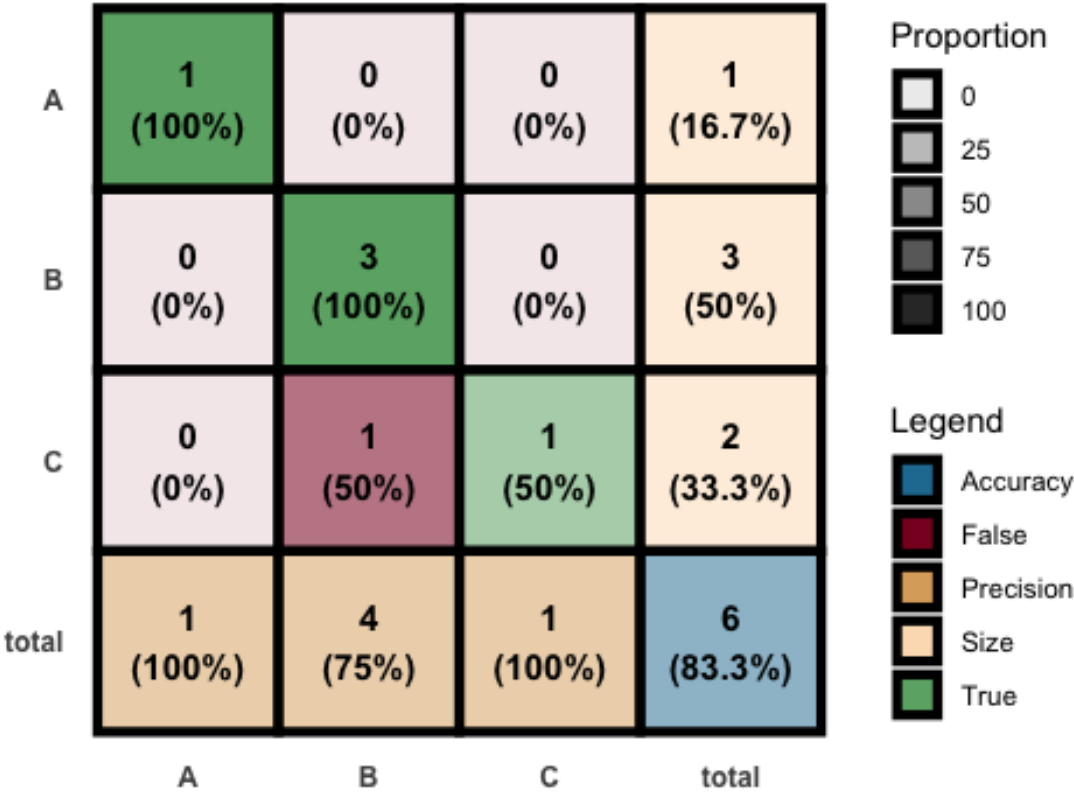
Training Set

Probability Heatmap



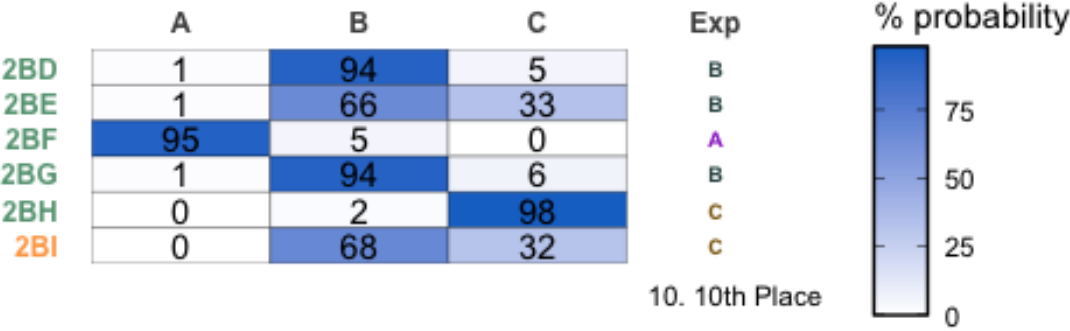
External Validation

Confusion Matrix



External Validation

Probability Heatmap



Section Results Summary

Error in eval(expr, envir, enclos): object 'model.sum.1' not found