

CH Activation - Model Testing - Stereoelectronic Features

Table of Contents

Truncated Datasets - Union of Similarity within Groups and with Group 3	1
Section Results Summary	1
1st Place.....	2
2nd Place.....	7
3rd Place.....	12
4th Place.....	17
5th Place.....	22
6th Place.....	27
7th Place.....	32
8th Place.....	37
9th Place.....	42
10th Place.....	47

Truncated Datasets - Union of Similarity within Groups and with Group 3

formula	McFadden R2
class ~ NPA_13 + diff_10_Metalla + dip_z_1 + Dist.9..13.	0.922
class ~ NPA_3 + diff_10_Metalla + dip_z_1 + Dist.9..13.	0.880
class ~ NPA_13 + NPA_Metallic + dip_z_1 + Dist.9..13.	0.865
class ~ NPA_4 + diff_9_Metalla + Total_1 + Dist.9..13.	0.846
class ~ diff_3_9 + diff_9_Metalla + dip_y_1 + Dist.9..13.	0.841
class ~ diff_3_4 + diff_10_Metalla + dip_z_1 + Dist.9..13.	0.836
class ~ NPA_4 + diff_9_Metalla + dip_y_1 + Dist.9..13.	0.827
class ~ diff_9_13 + diff_10_Metalla + dip_z_1 + Dist.9..13.	0.816
class ~ diff_10_Metalla + dip_z_1 + Dist.9..13. + Dist.3..9.	0.816
class ~ diff_3_9 + diff_10_Metalla + dip_z_1 + Dist.9..13.	0.812

Section Results Summary

	Training.Accuracy	Test.Accuracy
1. 1st Place	95.65	64.3
2. 2nd Place	95.65	71.4
3. 3rd Place	93.48	57.1
4. 4th Place	89.13	64.3
5. 5th Place	89.13	64.3
6. 6th Place	93.48	78.6
7. 7th Place	89.13	78.6
8. 8th Place	91.30	78.6

	Training.Accuracy	Test.Accuracy
9. 9th Place	89.13	64.3
10. 10th Place	91.30	78.6

1st Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
95.65%	0.922

Model Coefficients

	(Intercept)	NPA_13	diff_10_Metalla	dip_z_1	Dist.9..13.
2	995.50923	221.7893	-297.9995	15.649504	-533.70792
3	15.34703	209.5780	444.4071	-4.862628	-202.94310
4	-112.97499	185.4074	306.0002	-5.454354	-13.60712

Training Set

Confusion Matrix




1	10 (100%)	0 (0%)	0 (0%)	0 (0%)	10 (21.7%)
2	0 (0%)	13 (100%)	0 (0%)	0 (0%)	13 (28.3%)
3	0 (0%)	0 (0%)	9 (90%)	1 (10%)	10 (21.7%)
4	0 (0%)	0 (0%)	1 (7.7%)	12 (92.3%)	13 (28.3%)
total	10 (100%)	13 (100%)	10 (90%)	13 (92.3%)	46 (95.7%)
	1	2	3	4	total

1. 1st Place

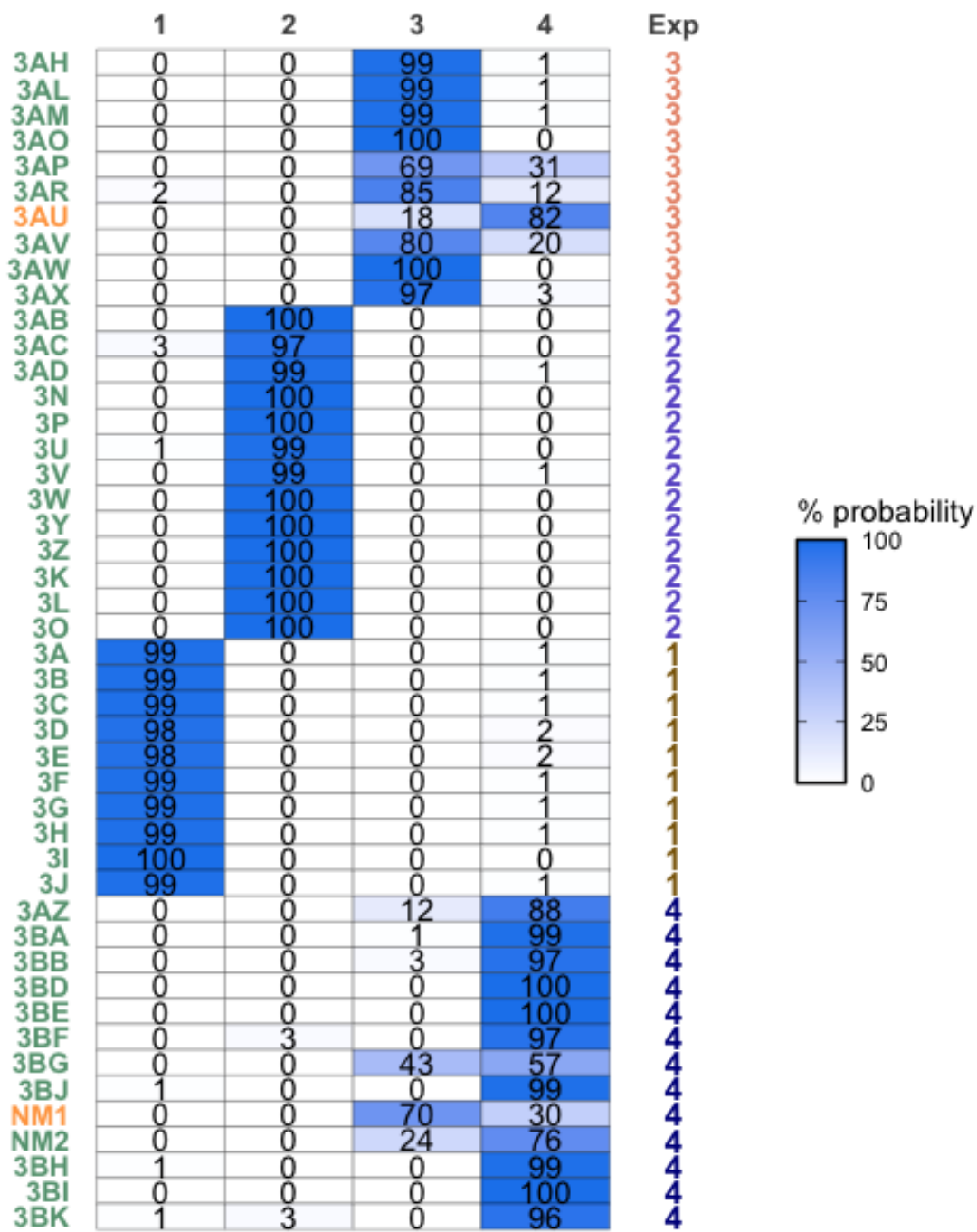
Legend

	Accuracy
	False
	Precision
	Size
	True

prop

	0
	25
	50
	75
	100

Training Set Probability Heatmap



1. 1st Place

Test Set

Confusion Matrix

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	1 (20%)	4 (80%)	0 (0%)	0 (0%)	5 (35.7%)
3	0 (0%)	0 (0%)	5 (62.5%)	3 (37.5%)	8 (57.1%)
4	0 (0%)	0 (0%)	1 (100%)	0 (0%)	1 (7.1%)
total	1 (0%)	4 (100%)	6 (83.3%)	3 (0%)	14 (64.3%)
	1	2	3	4	total

1. 1st Place

Legend

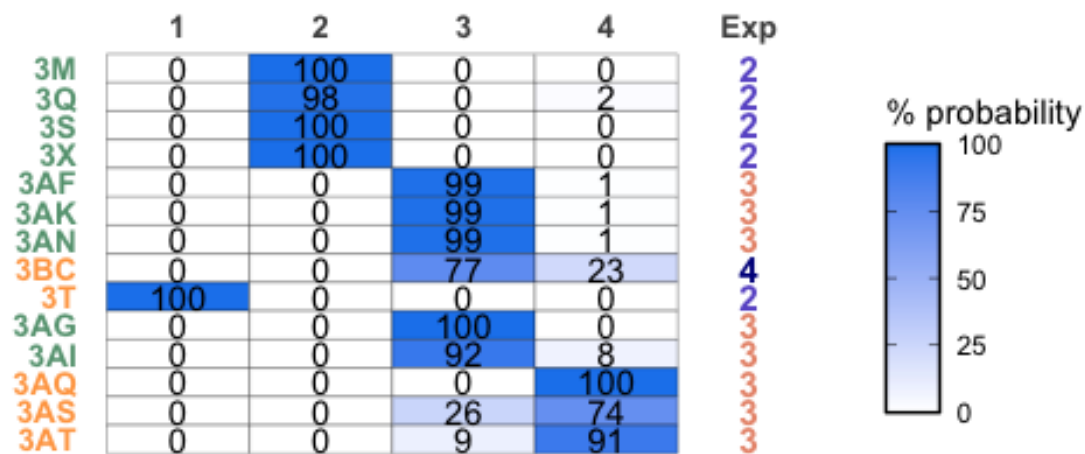
- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Test Set

Probability Heatmap



1. 1st Place

2nd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
95.65%	0.88

Model Coefficients

	(Intercept)	NPA_3	diff_10_Metalla	dip_z_1	Dist.9..13.
2	805.57490	75.532694	-402.97645	15.0219919	-402.01222
3	362.48829	392.722698	607.45946	-0.7748407	-669.39737
4	-80.42359	-3.776181	48.35616	-2.4597382	33.96917

Training Set



Confusion Matrix

1	10 (100%)	0 (0%)	0 (0%)	0 (0%)	10 (21.7%)
2	0 (0%)	13 (100%)	0 (0%)	0 (0%)	13 (28.3%)
3	0 (0%)	0 (0%)	10 (100%)	0 (0%)	10 (21.7%)
4	2 (15.4%)	0 (0%)	0 (0%)	11 (84.6%)	13 (28.3%)
total	12 (83.3%)	13 (100%)	10 (100%)	11 (100%)	46 (95.7%)
	1	2	3	4	total

Legend

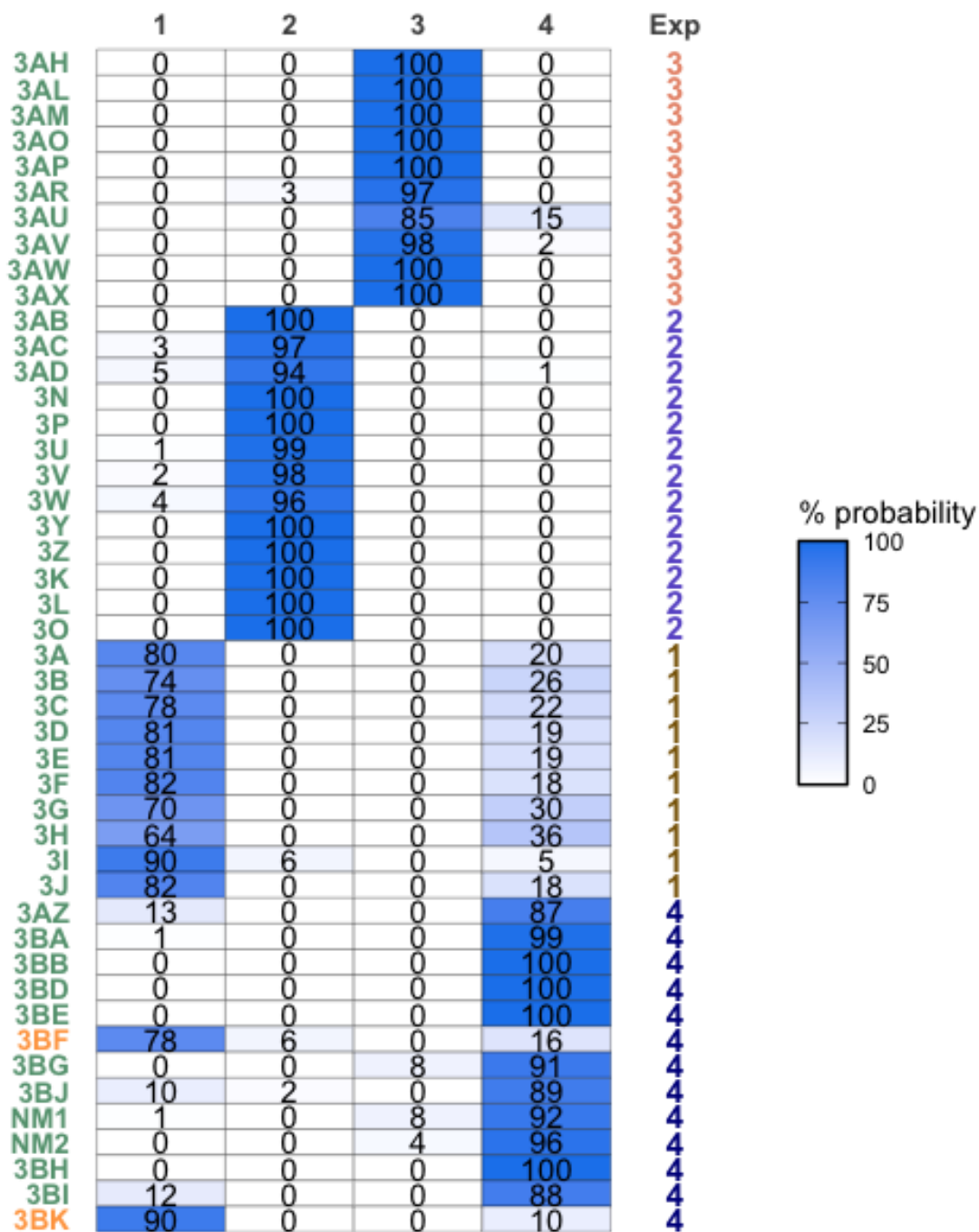
	Accuracy
	False
	Precision
	Size
	True

prop

	0
	25
	50
	75
	100

2. 2nd Place

Training Set Probability Heatmap



2. 2nd Place

Test Set

Confusion Matrix

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	2 (40%)	3 (60%)	0 (0%)	0 (0%)	5 (35.7%)
3	0 (0%)	0 (0%)	6 (75%)	2 (25%)	8 (57.1%)
4	0 (0%)	0 (0%)	0 (0%)	1 (100%)	1 (7.1%)
total	2 (0%)	3 (100%)	6 (100%)	3 (33.3%)	14 (71.4%)
	1	2	3	4	total

Legend

- Accuracy
- False
- Precision
- Size
- True

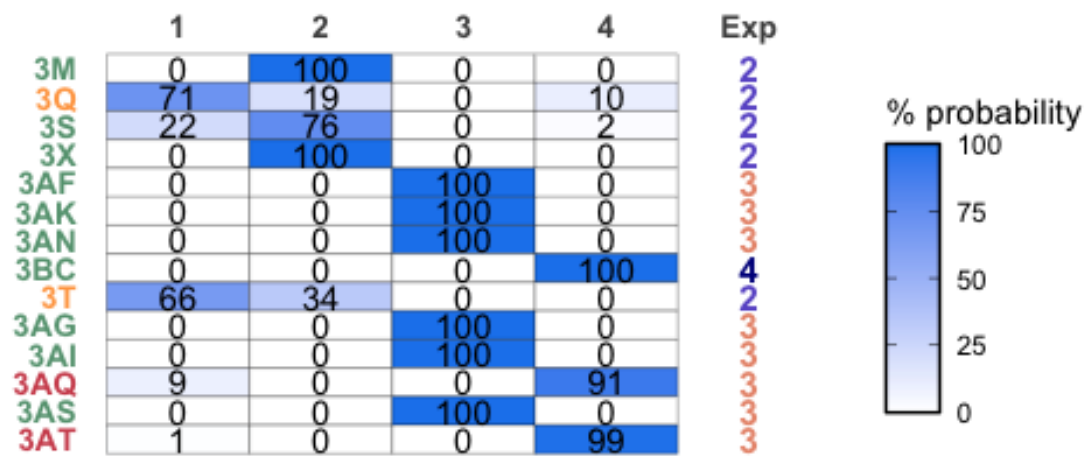
prop

- 0
- 25
- 50
- 75
- 100

2. 2nd Place

Test Set

Probability Heatmap



2. 2nd Place

3rd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
93.48%	0.865

Model Coefficients

	(Intercept)	NPA_13	NPA_Metallic	dip_z_1	Dist.9..13.
2	1023.003931	200.9343	427.8298	19.564621	-569.28253
3	242.967137	196.9562	-421.3641	-1.717786	-306.68032
4	-1.981098	158.9234	-200.6125	-2.994236	-15.00583

Training Set

Confusion Matrix

1	10 (100%)	0 (0%)	0 (0%)	0 (0%)	10 (21.7%)
2	1 (7.7%)	12 (92.3%)	0 (0%)	0 (0%)	13 (28.3%)
3	0 (0%)	0 (0%)	9 (90%)	1 (10%)	10 (21.7%)
4	0 (0%)	0 (0%)	1 (7.7%)	12 (92.3%)	13 (28.3%)
total	11 (90.9%)	12 (100%)	10 (90%)	13 (92.3%)	46 (93.5%)
	1	2	3	4	total

3. 3rd Place

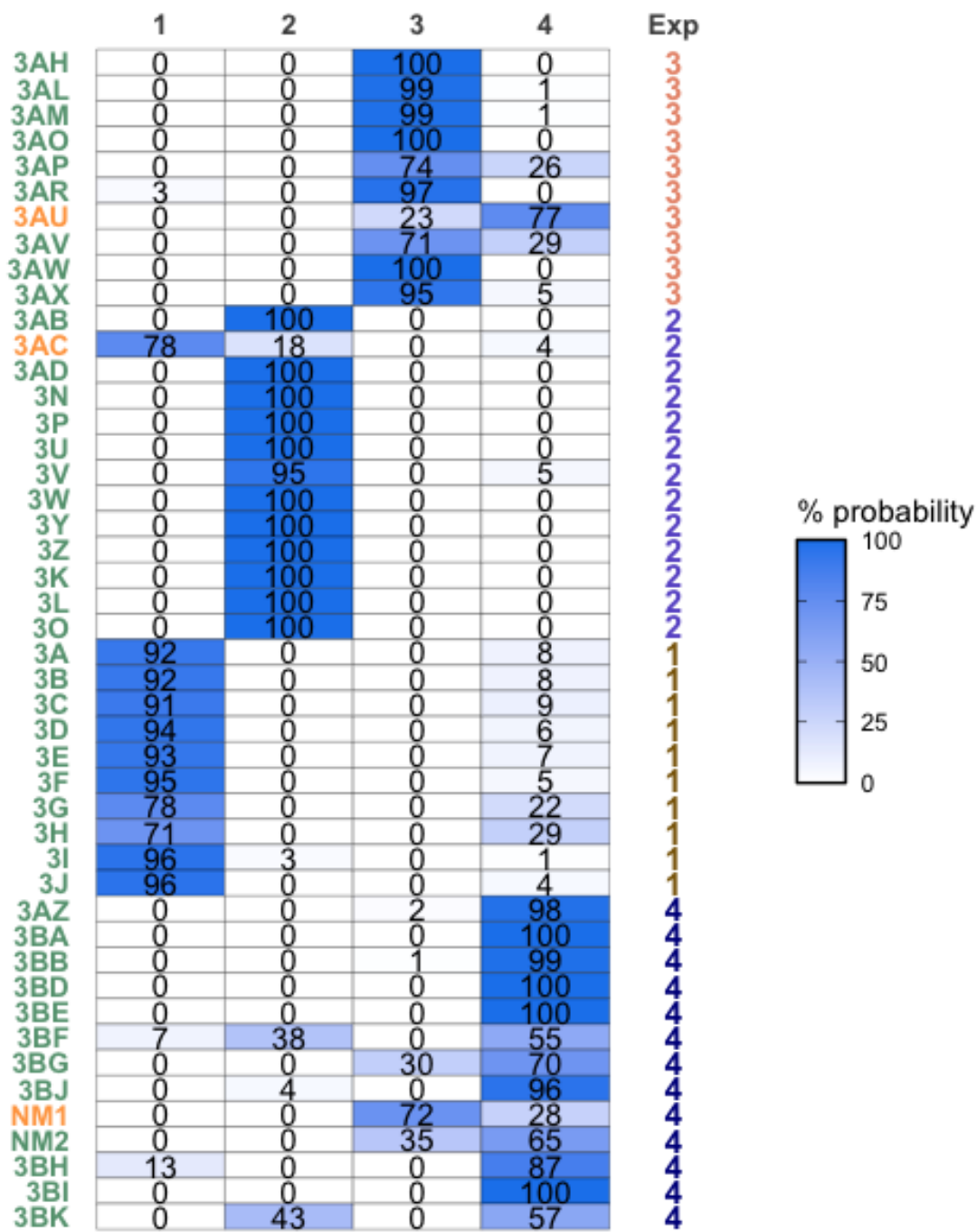
Legend

- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Training Set Probability Heatmap



3. 3rd Place

Test Set

Confusion Matrix

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	1 (20%)	4 (80%)	0 (0%)	0 (0%)	5 (35.7%)
3	0 (0%)	0 (0%)	4 (50%)	4 (50%)	8 (57.1%)
4	0 (0%)	0 (0%)	1 (100%)	0 (0%)	1 (7.1%)
total	1 (0%)	4 (100%)	5 (80%)	4 (0%)	14 (57.1%)
	1	2	3	4	total

3. 3rd Place

Legend

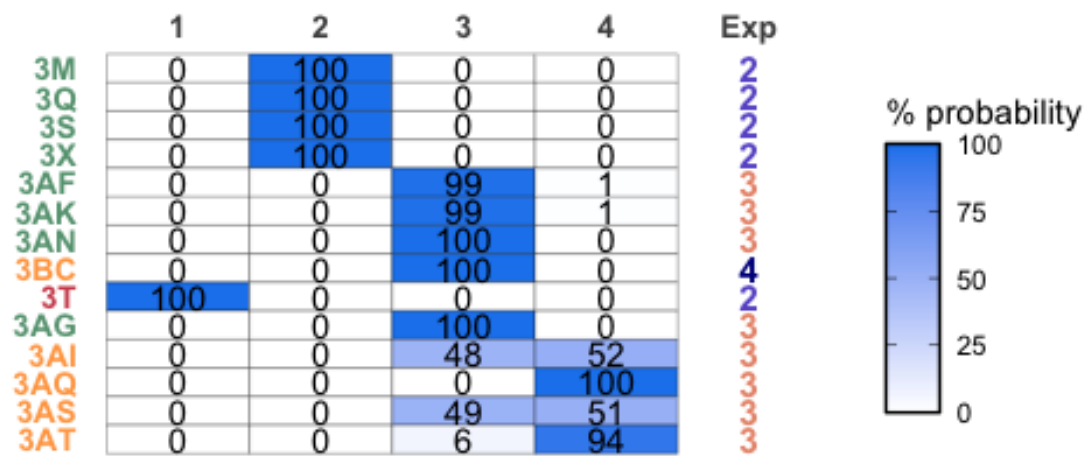
- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Test Set

Probability Heatmap



3. 3rd Place

4th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
89.13%	0.846

Model Coefficients

	(Intercept)	NPA_4	diff_9_Metalla	Total_1	Dist.9..13.
2	1027.29076	153.2190	-128.688501	-16.3937804	-673.58403
3	38.06996	-850.2408	10.128512	-3.7127652	-144.44633
4	-59.69783	-173.9114	9.751767	0.8863917	15.06327

Training Set

Confusion Matrix

1	7 (70%)	0 (0%)	0 (0%)	3 (30%)	10 (21.7%)
2	0 (0%)	13 (100%)	0 (0%)	0 (0%)	13 (28.3%)
3	0 (0%)	0 (0%)	10 (100%)	0 (0%)	10 (21.7%)
4	2 (15.4%)	0 (0%)	0 (0%)	11 (84.6%)	13 (28.3%)
total	9 (77.8%)	13 (100%)	10 (100%)	14 (78.6%)	46 (89.1%)
	1	2	3	4	total

4. 4th Place

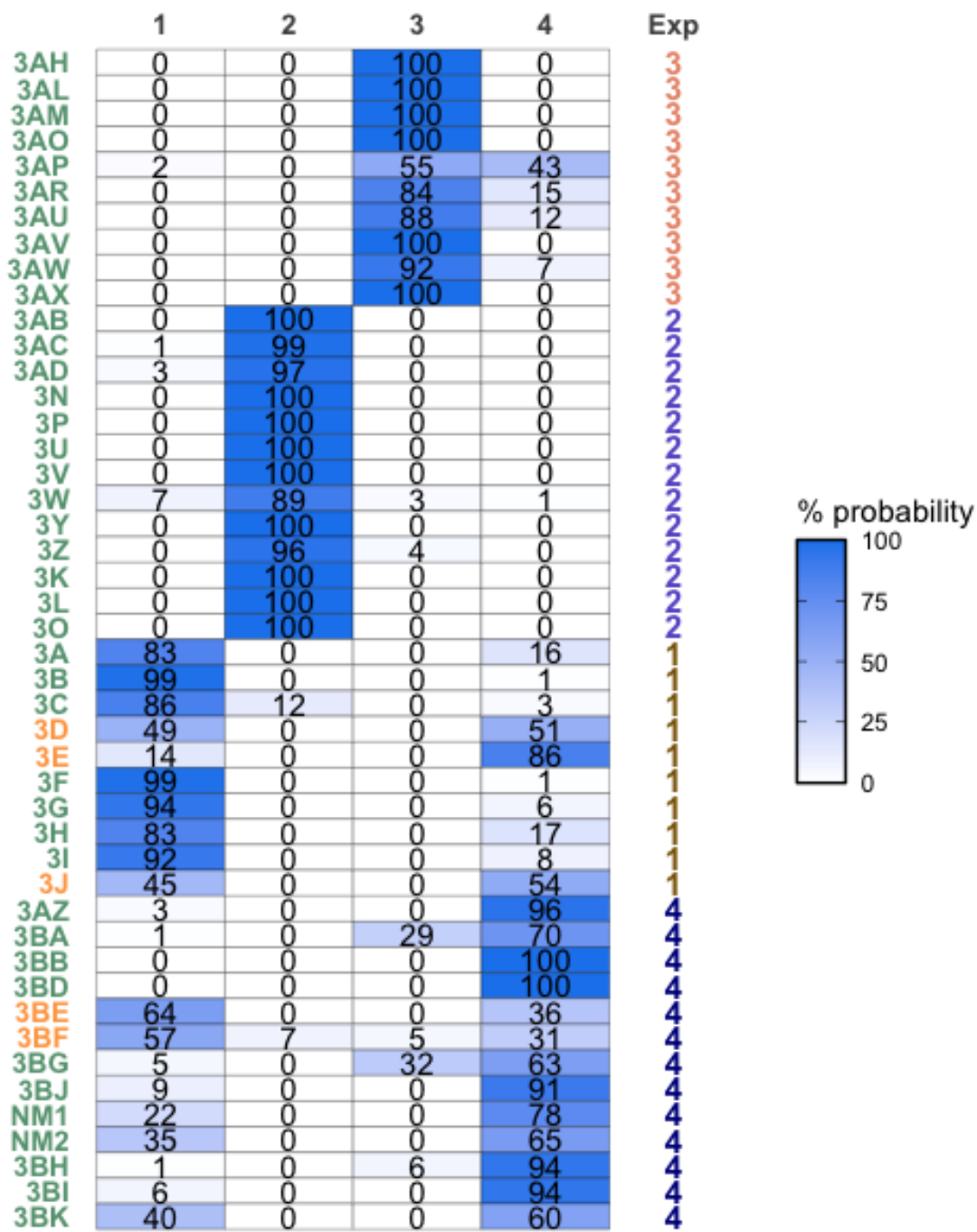
Legend

- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Training Set Probability Heatmap



4. 4th Place

Test Set

Confusion Matrix

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	2 (40%)	2 (40%)	0 (0%)	1 (20%)	5 (35.7%)
3	0 (0%)	0 (0%)	6 (75%)	2 (25%)	8 (57.1%)
4	0 (0%)	0 (0%)	0 (0%)	1 (100%)	1 (7.1%)
total	2 (0%)	2 (100%)	6 (100%)	4 (25%)	14 (64.3%)
	1	2	3	4	total

4. 4th Place

Legend

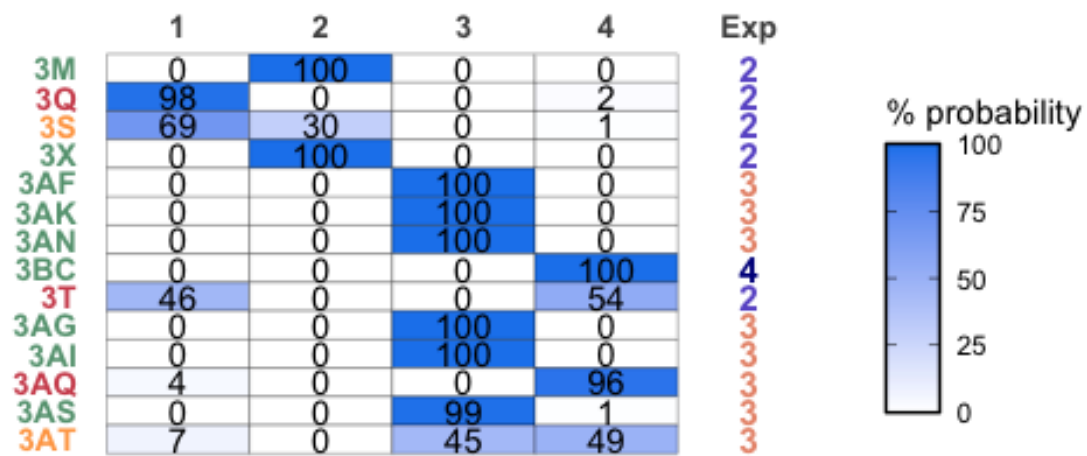
- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Test Set

Probability Heatmap



4. 4th Place

5th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
89.13%	0.841

Model Coefficients

	(Intercept)	diff_3_9	diff_9_Metalla	dip_y_1	Dist.9..13.
2	260.57896	3.706763	-25.32449	1.748104	-187.1860
3	56.37232	-457.853633	500.44074	-13.960238	-286.4973
4	-259.91049	-88.659880	110.08077	-7.980223	151.8795

Training Set





Confusion Matrix

1	8 (80%)	1 (10%)	0 (0%)	1 (10%)	10 (21.7%)
2	1 (7.7%)	12 (92.3%)	0 (0%)	0 (0%)	13 (28.3%)
3	0 (0%)	0 (0%)	10 (100%)	0 (0%)	10 (21.7%)
4	0 (0%)	1 (7.7%)	1 (7.7%)	11 (84.6%)	13 (28.3%)
total	9 (88.9%)	14 (85.7%)	11 (90.9%)	12 (91.7%)	46 (89.1%)
	1	2	3	4	total

Legend

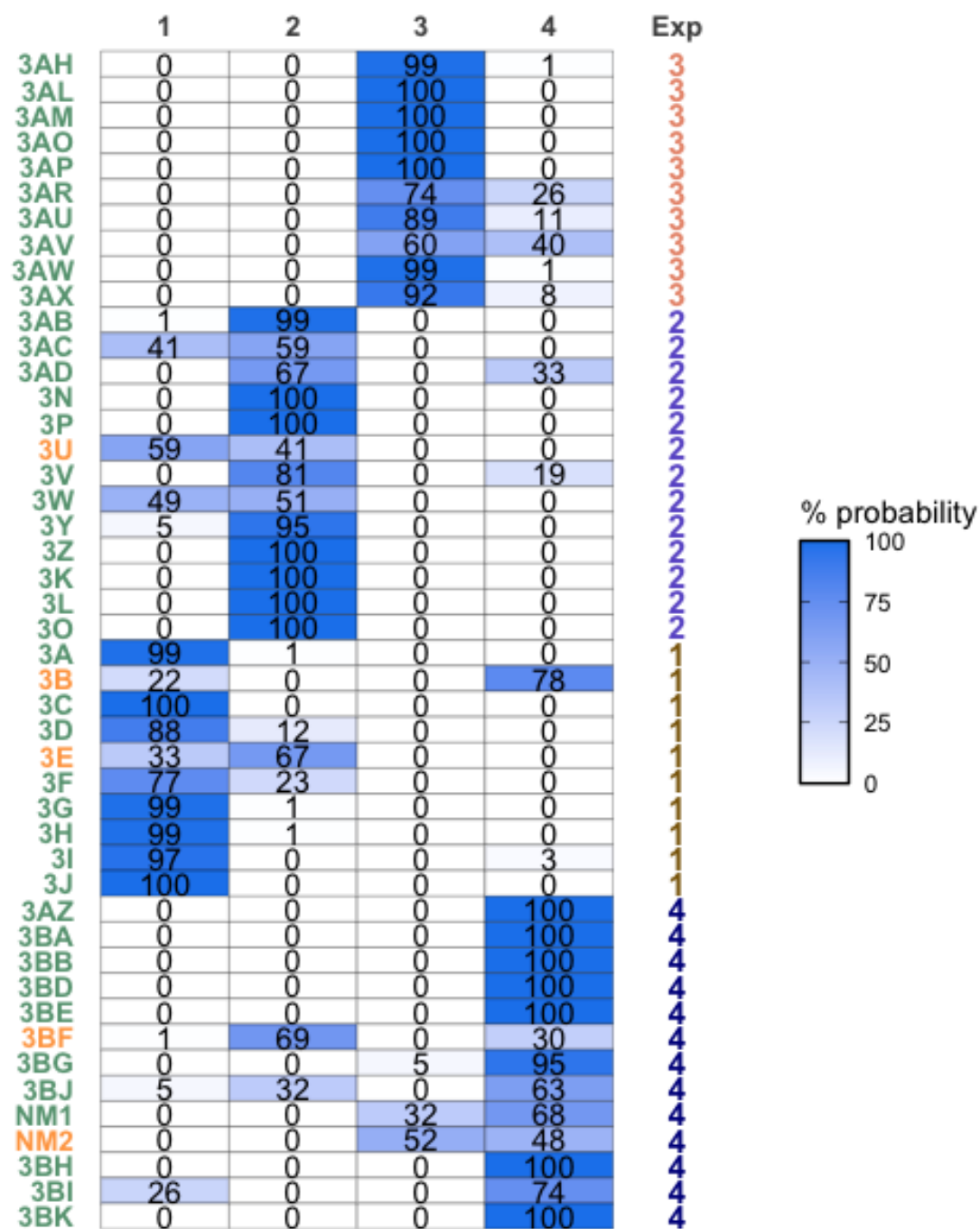
	Accuracy
	False
	Precision
	Size
	True

prop

	0
	25
	50
	75
	100

5. 5th Place

Training Set Probability Heatmap



5. 5th Place

Test Set

Confusion Matrix

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	0 (0%)	3 (60%)	0 (0%)	2 (40%)	5 (35.7%)
3	0 (0%)	0 (0%)	5 (62.5%)	3 (37.5%)	8 (57.1%)
4	0 (0%)	0 (0%)	0 (0%)	1 (100%)	1 (7.1%)
total	0 (0%)	3 (100%)	5 (100%)	6 (16.7%)	14 (64.3%)
	1	2	3	4	total

5. 5th Place

Legend

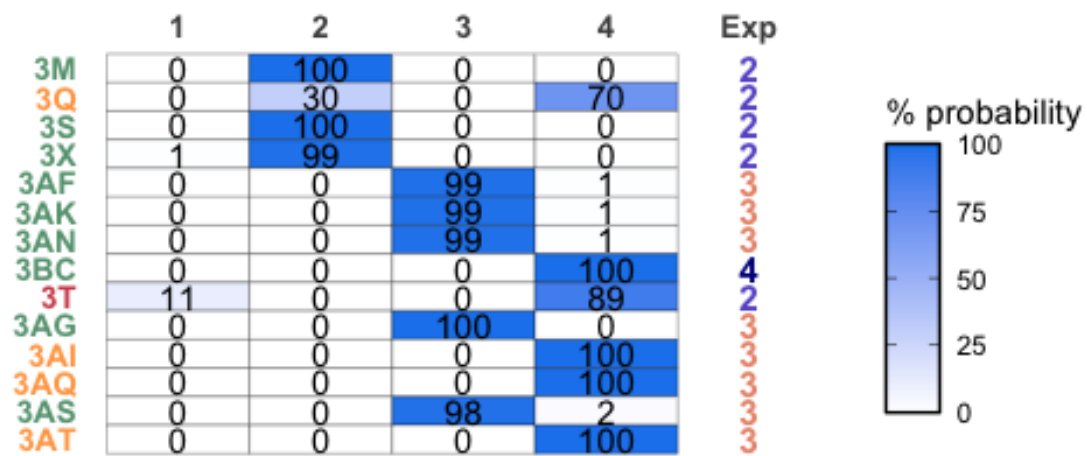
- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Test Set

Probability Heatmap



5. 5th Place

6th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
93.48%	0.836

Model Coefficients

	(Intercept)	diff_3_4	diff_10_Metalla	dip_z_1	Dist.9..13.
2	543.51660	31.208967	-298.90181	10.818354	-260.63675
3	257.54864	292.993026	512.54426	-1.060874	-569.28247
4	-80.02205	-2.260941	48.93302	-2.487356	33.74686

Training Set

Confusion Matrix

1	9 (90%)	1 (10%)	0 (0%)	0 (0%)	10 (21.7%)
2	0 (0%)	13 (100%)	0 (0%)	0 (0%)	13 (28.3%)
3	0 (0%)	0 (0%)	10 (100%)	0 (0%)	10 (21.7%)
4	2 (15.4%)	0 (0%)	0 (0%)	11 (84.6%)	13 (28.3%)
total	11 (81.8%)	14 (92.9%)	10 (100%)	11 (100%)	46 (93.5%)
	1	2	3	4	total

6. 6th Place

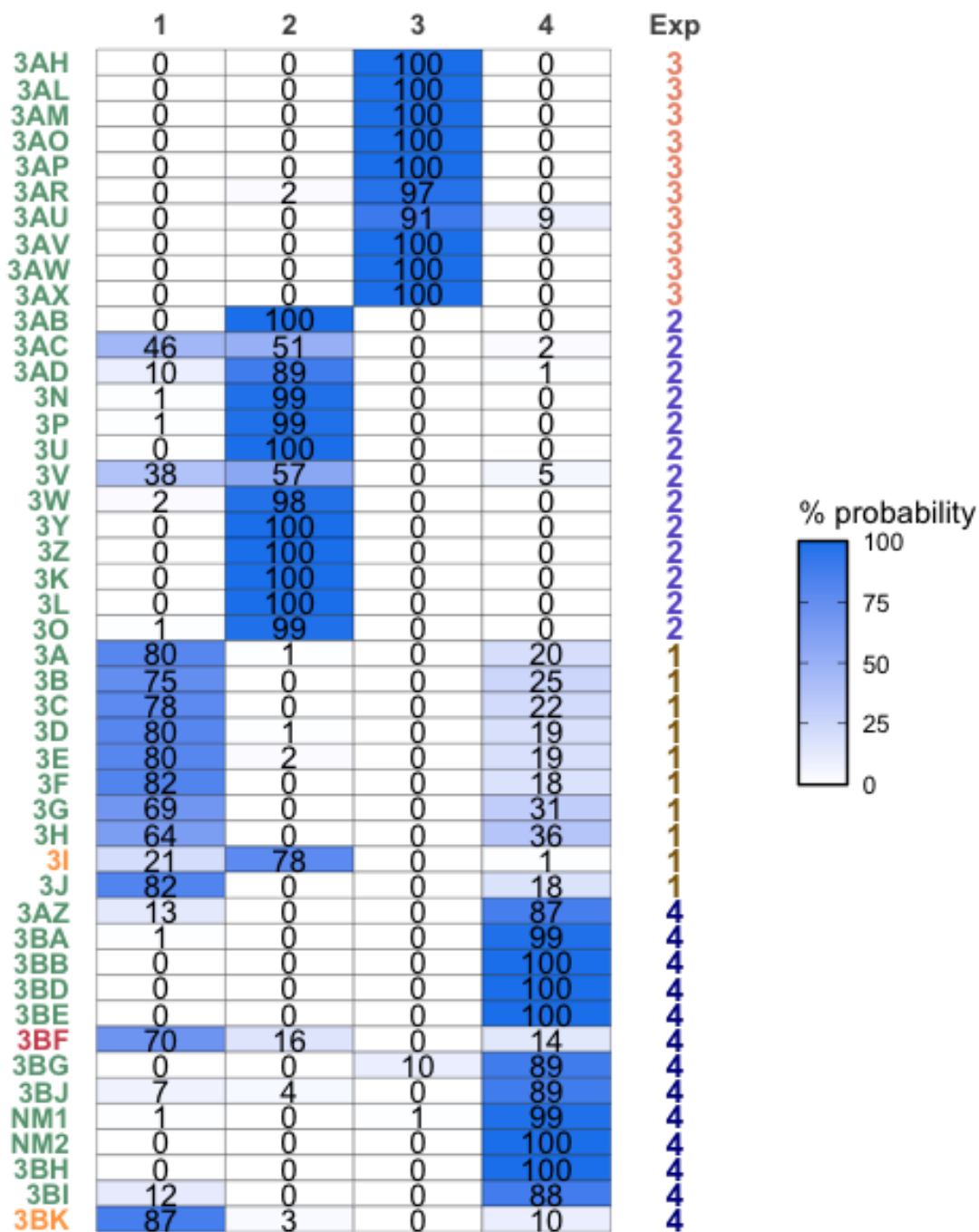
Legend

- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Training Set Probability Heatmap



6. 6th Place

Test Set

Confusion Matrix

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	1 (20%)	4 (80%)	0 (0%)	0 (0%)	5 (35.7%)
3	0 (0%)	0 (0%)	6 (75%)	2 (25%)	8 (57.1%)
4	0 (0%)	0 (0%)	0 (0%)	1 (100%)	1 (7.1%)
total	1 (0%)	4 (100%)	6 (100%)	3 (33.3%)	14 (78.6%)
	1	2	3	4	total

6. 6th Place

Legend

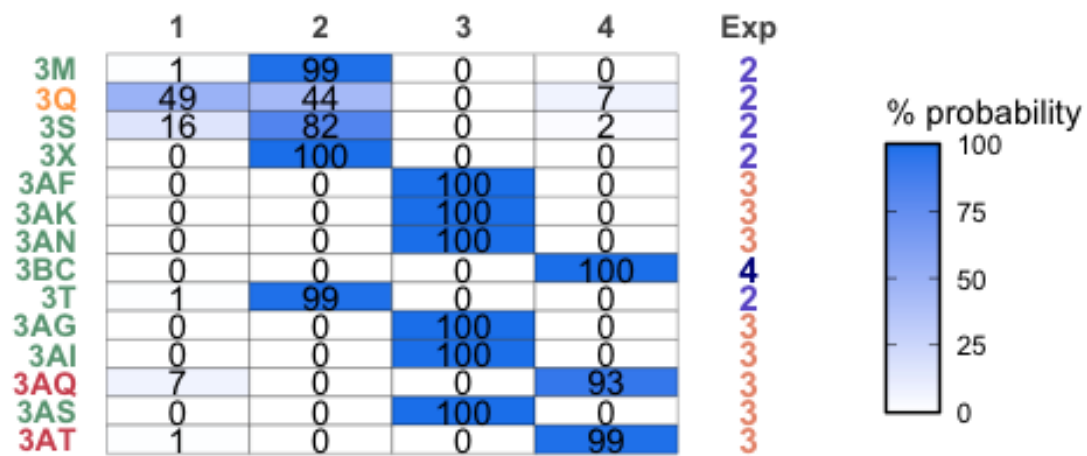
- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Test Set

Probability Heatmap



6. 6th Place

7th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
89.13%	0.827

Model Coefficients

	(Intercept)	NPA_4	diff_9_Metalla	dip_y_1	Dist.9..13.
2	243.8525	17.62842	-19.66997	1.010868	-173.9379
3	-731.6367	-1106.15560	94.82302	-12.856340	346.9258
4	-753.0084	-874.13914	92.92296	-12.939813	398.4610

Training Set

Confusion Matrix

1	9 (90%)	0 (0%)	0 (0%)	1 (10%)	10 (21.7%)
2	0 (0%)	13 (100%)	0 (0%)	0 (0%)	13 (28.3%)
3	0 (0%)	0 (0%)	9 (90%)	1 (10%)	10 (21.7%)
4	1 (7.7%)	1 (7.7%)	1 (7.7%)	10 (76.9%)	13 (28.3%)
total	10 (90%)	14 (92.9%)	10 (90%)	12 (83.3%)	46 (89.1%)
	1	2	3	4	total

7. 7th Place

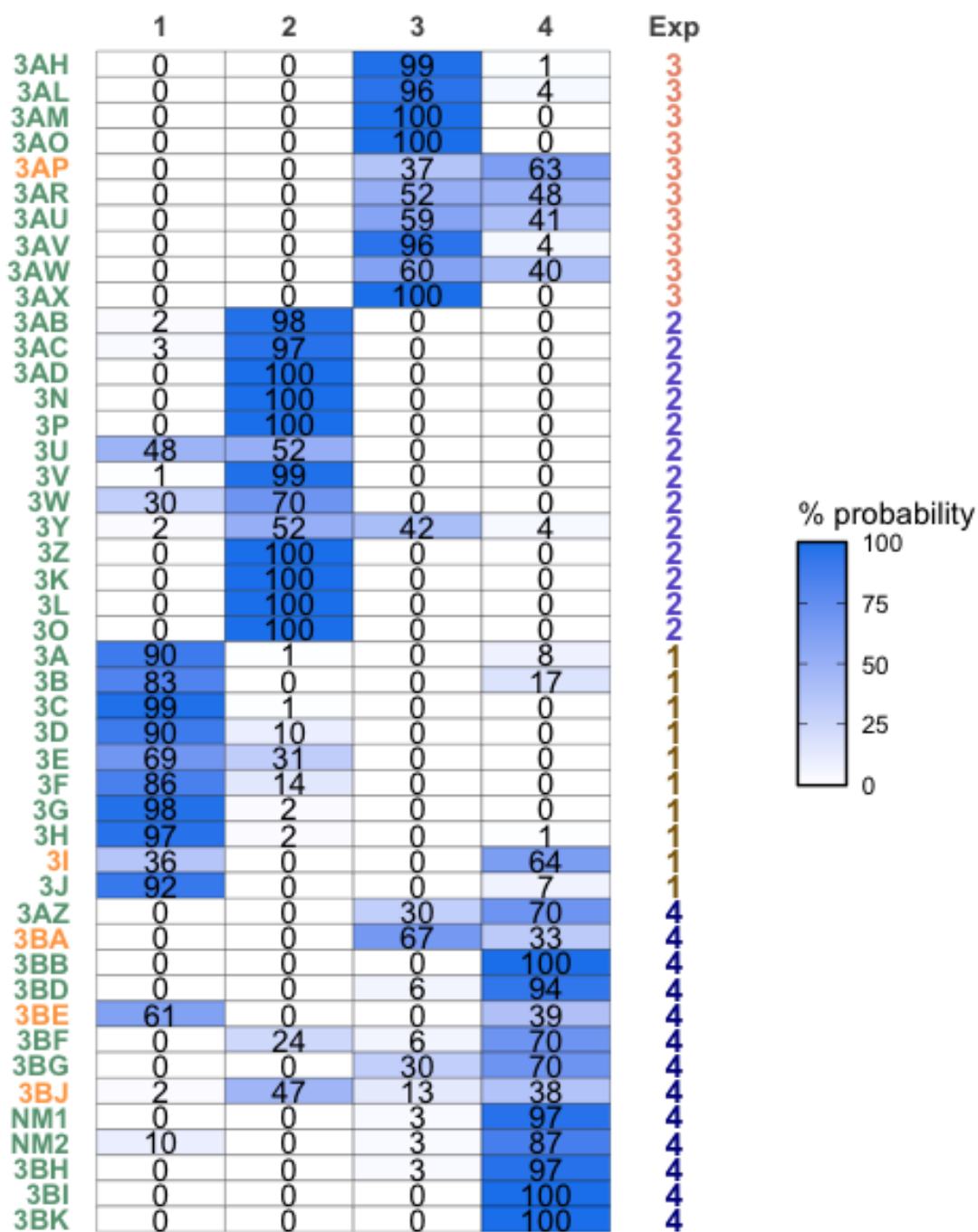
Legend

- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Training Set Probability Heatmap



7. 7th Place

Test Set

Confusion Matrix

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	0 (0%)	4 (80%)	0 (0%)	1 (20%)	5 (35.7%)
3	0 (0%)	0 (0%)	6 (75%)	2 (25%)	8 (57.1%)
4	0 (0%)	0 (0%)	0 (0%)	1 (100%)	1 (7.1%)
total	0 (0%)	4 (100%)	6 (100%)	4 (25%)	14 (78.6%)
	1	2	3	4	total

7. 7th Place

Legend

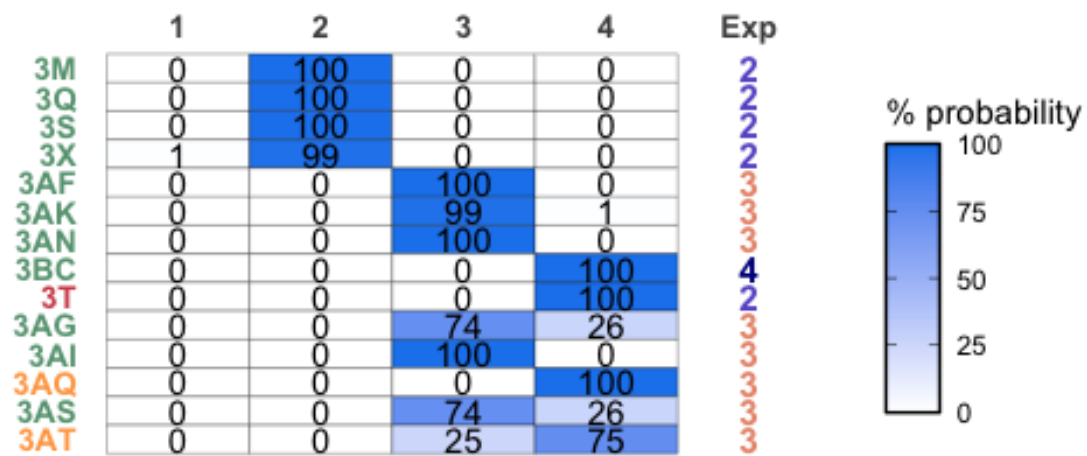
- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Test Set

Probability Heatmap



7. 7th Place

8th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
91.3%	0.816

Model Coefficients




	(Intercept)	diff_9_13	diff_10_Metalla	dip_z_1	Dist.9..13.
2	858.02659	-20.202345	-415.85856	15.0485288	-428.70703
3	64.05685	-13.535248	143.24162	-0.7661797	-135.32271
4	-29.54426	-4.288104	41.01538	-1.6637645	2.08915

Training Set


Confusion Matrix

1	10 (100%)	0 (0%)	0 (0%)	0 (0%)	10 (21.7%)
2	0 (0%)	13 (100%)	0 (0%)	0 (0%)	13 (28.3%)
3	0 (0%)	0 (0%)	9 (90%)	1 (10%)	10 (21.7%)
4	2 (15.4%)	0 (0%)	1 (7.7%)	10 (76.9%)	13 (28.3%)
total	12 (83.3%)	13 (100%)	10 (90%)	11 (90.9%)	46 (91.3%)
	1	2	3	4	total

Legend

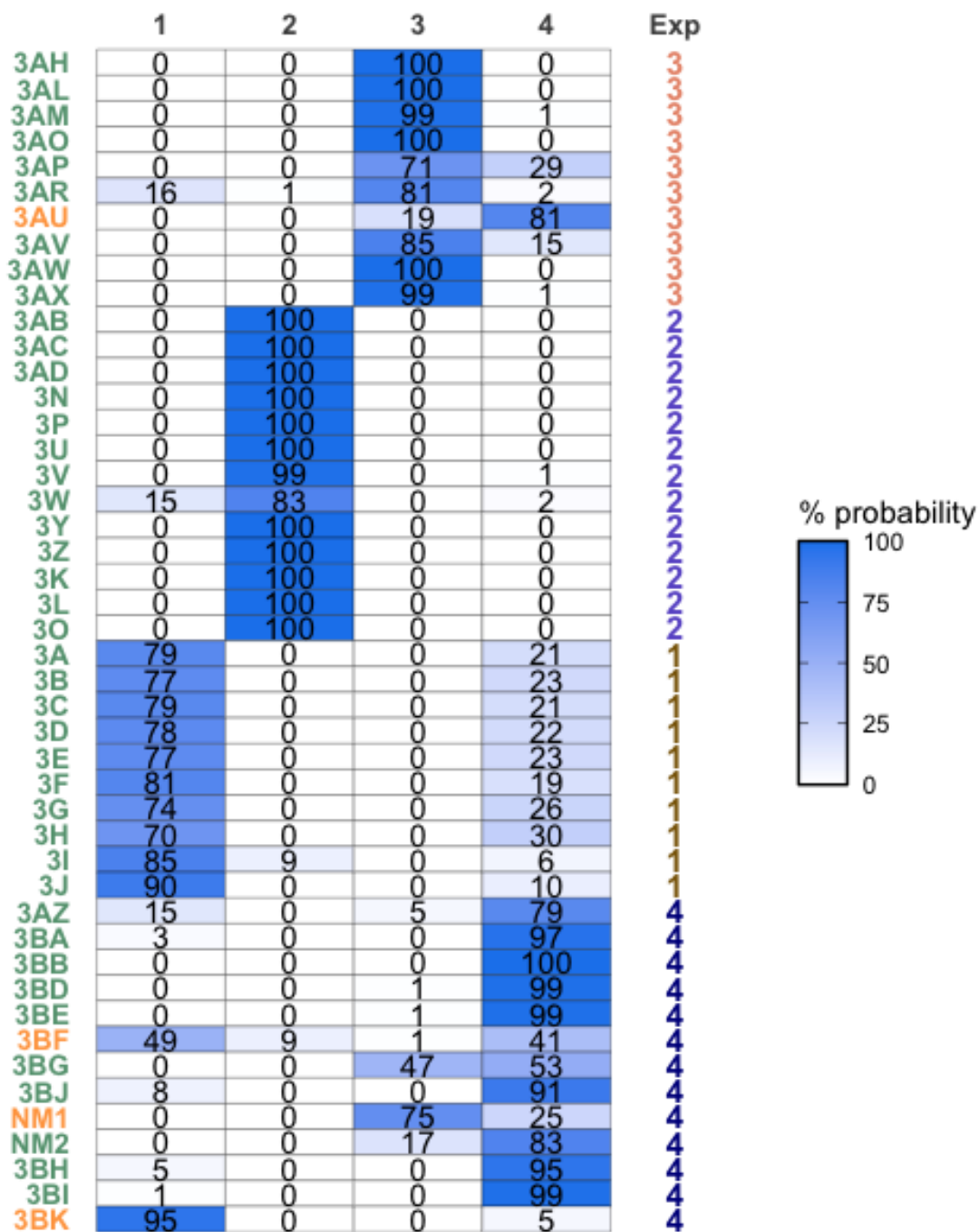
	Accuracy
	False
	Precision
	Size
	True

prop

	0
	25
	50
	75
	100

8. 8th Place

Training Set Probability Heatmap







8. 8th Place

Test Set






Confusion Matrix

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	0 (0%)	5 (100%)	0 (0%)	0 (0%)	5 (35.7%)
3	0 (0%)	0 (0%)	5 (62.5%)	3 (37.5%)	8 (57.1%)
4	0 (0%)	0 (0%)	0 (0%)	1 (100%)	1 (7.1%)
total	0 (0%)	5 (100%)	5 (100%)	4 (25%)	14 (78.6%)
	1	2	3	4	total

Legend

	Accuracy
	False
	Precision
	Size
	True

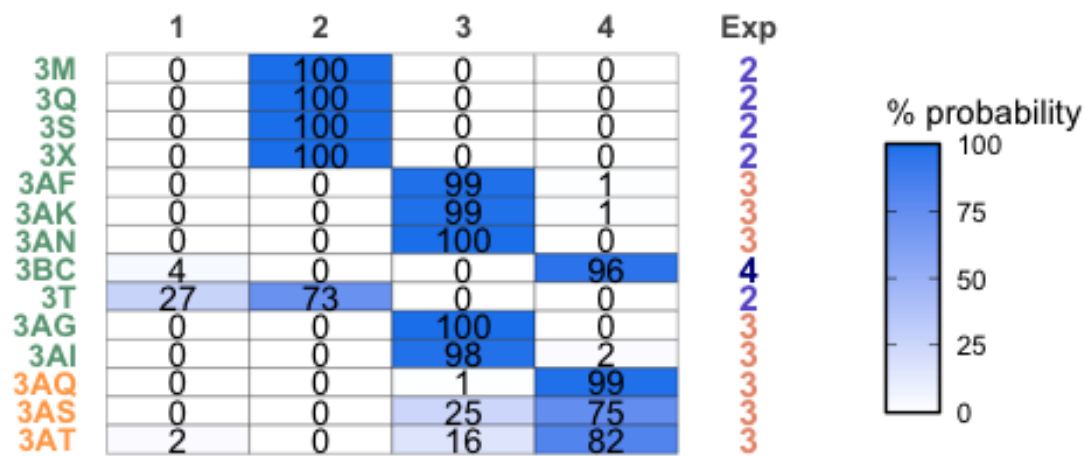
prop

	0
	25
	50
	75
	100

8. 8th Place

Test Set

Probability Heatmap



8. 8th Place

9th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
89.13%	0.816

Model Coefficients

	(Intercept)	diff_10_Metalla	dip_z_1	Dist.9..13.	Dist.3..9.
2	649.1959	-207.96181	7.526964	-215.56516	-153.71759
3	-186.7019	194.37583	-3.893152	-10.85198	30.92951
4	-344.3557	91.93223	-5.411500	47.26975	144.91266

Training Set




Confusion Matrix

1	8 (80%)	1 (10%)	0 (0%)	1 (10%)	10 (21.7%)
2	0 (0%)	13 (100%)	0 (0%)	0 (0%)	13 (28.3%)
3	0 (0%)	0 (0%)	9 (90%)	1 (10%)	10 (21.7%)
4	1 (7.7%)	0 (0%)	1 (7.7%)	11 (84.6%)	13 (28.3%)
total	9 (88.9%)	14 (92.9%)	10 (90%)	13 (84.6%)	46 (89.1%)
	1	2	3	4	total

Legend

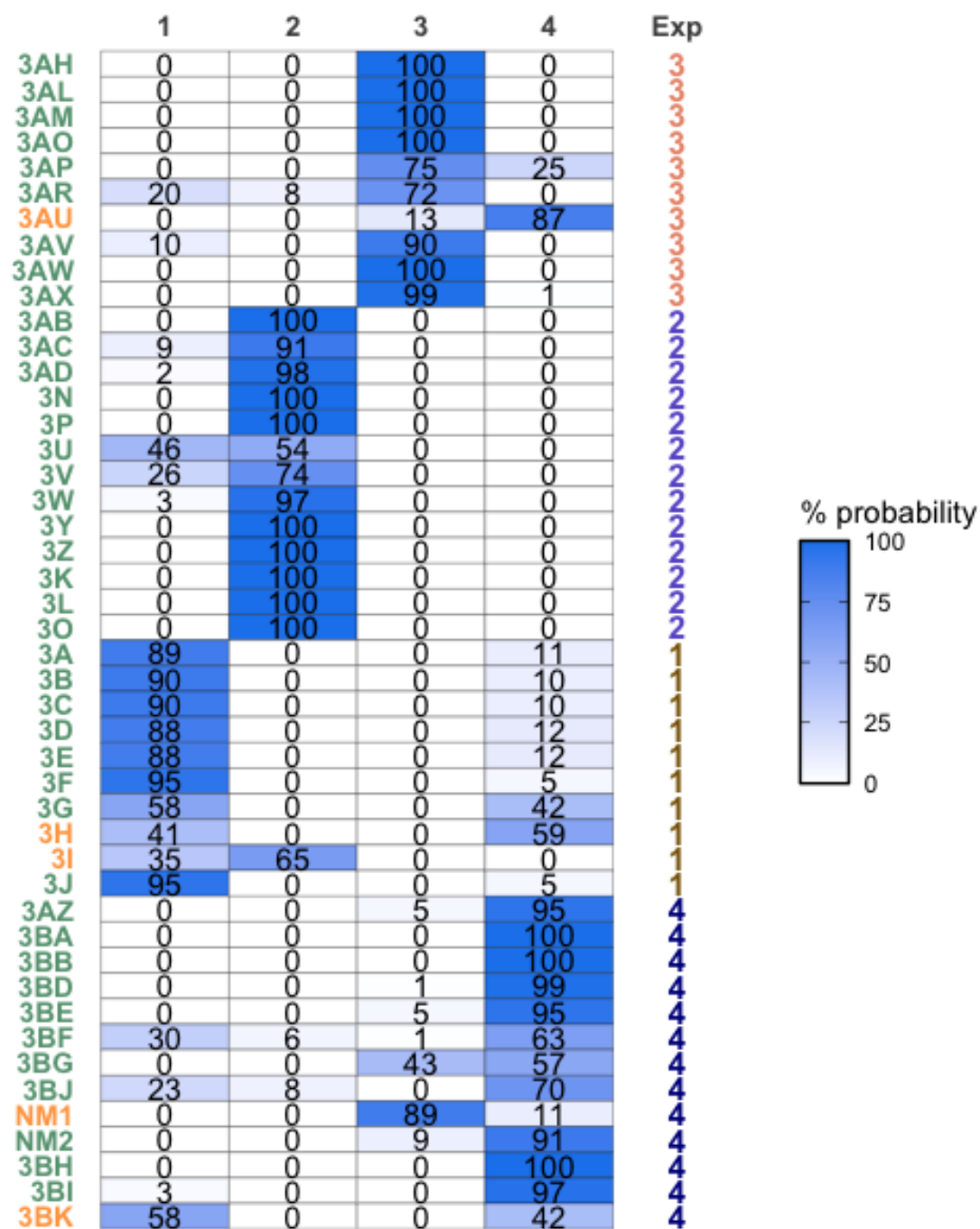
	Accuracy
	False
	Precision
	Size
	True

prop

	0
	25
	50
	75
	100

9. 9th Place

Training Set Probability Heatmap



9. 9th Place

Test Set

Confusion Matrix

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	1 (20%)	4 (80%)	0 (0%)	0 (0%)	5 (35.7%)
3	1 (12.5%)	0 (0%)	5 (62.5%)	2 (25%)	8 (57.1%)
4	0 (0%)	0 (0%)	1 (100%)	0 (0%)	1 (7.1%)
total	2 (0%)	4 (100%)	6 (83.3%)	2 (0%)	14 (64.3%)
	1	2	3	4	total

Legend

- Accuracy
- False
- Precision
- Size
- True

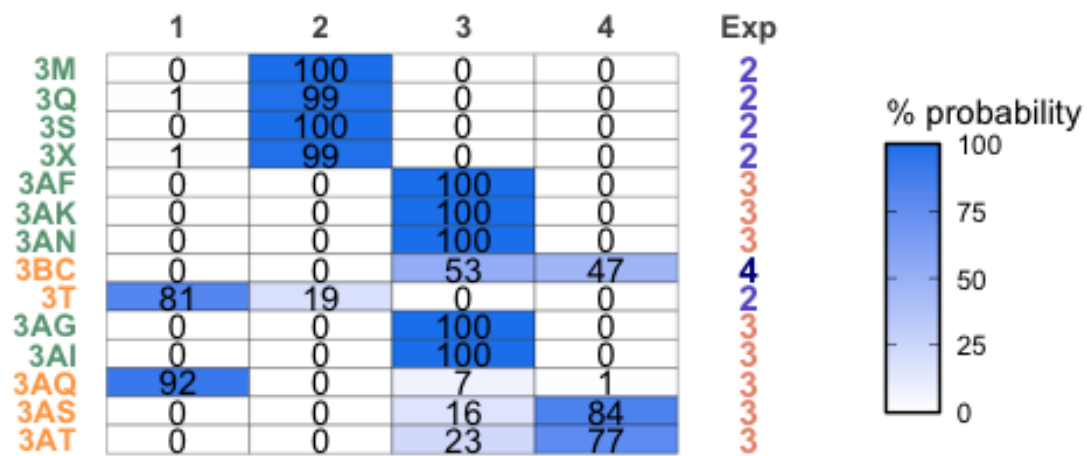
prop

- 0
- 25
- 50
- 75
- 100

9. 9th Place

Test Set

Probability Heatmap



9. 9th Place

10th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
91.3%	0.812

Model Coefficients

	(Intercept)	diff_3_9	diff_10_Metalla	dip_z_1	Dist.9..13.
2	869.14408	-24.7632774	-418.69237	15.428139	-439.62916
3	26.78698	-17.0976760	165.18908	-1.063142	-122.13931
4	-70.39020	0.3001565	45.36738	-2.090129	28.35965

Training Set



Confusion Matrix

1	10 (100%)	0 (0%)	0 (0%)	0 (0%)	10 (21.7%)
2	0 (0%)	13 (100%)	0 (0%)	0 (0%)	13 (28.3%)
3	0 (0%)	0 (0%)	9 (90%)	1 (10%)	10 (21.7%)
4	2 (15.4%)	0 (0%)	1 (7.7%)	10 (76.9%)	13 (28.3%)
total	12 (83.3%)	13 (100%)	10 (90%)	11 (90.9%)	46 (91.3%)
	1	2	3	4	total

Legend

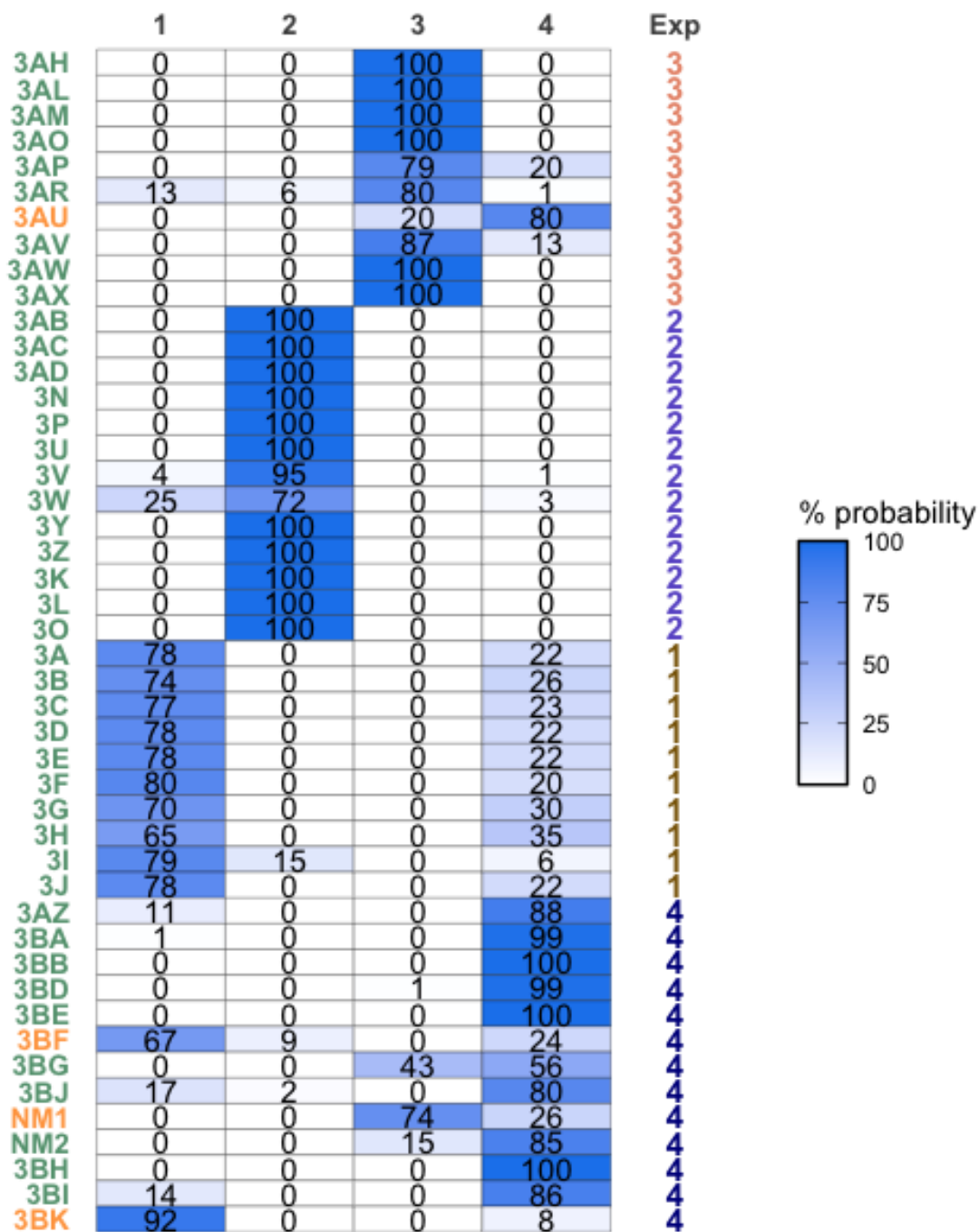
	Accuracy
	False
	Precision
	Size
	True

prop

	0
	25
	50
	75
	100

10. 10th Place

Training Set Probability Heatmap



10. 10th Place

Test Set

Confusion Matrix

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	0 (0%)	5 (100%)	0 (0%)	0 (0%)	5 (35.7%)
3	0 (0%)	0 (0%)	5 (62.5%)	3 (37.5%)	8 (57.1%)
4	0 (0%)	0 (0%)	0 (0%)	1 (100%)	1 (7.1%)
total	0 (0%)	5 (100%)	5 (100%)	4 (25%)	14 (78.6%)
	1	2	3	4	total

Legend

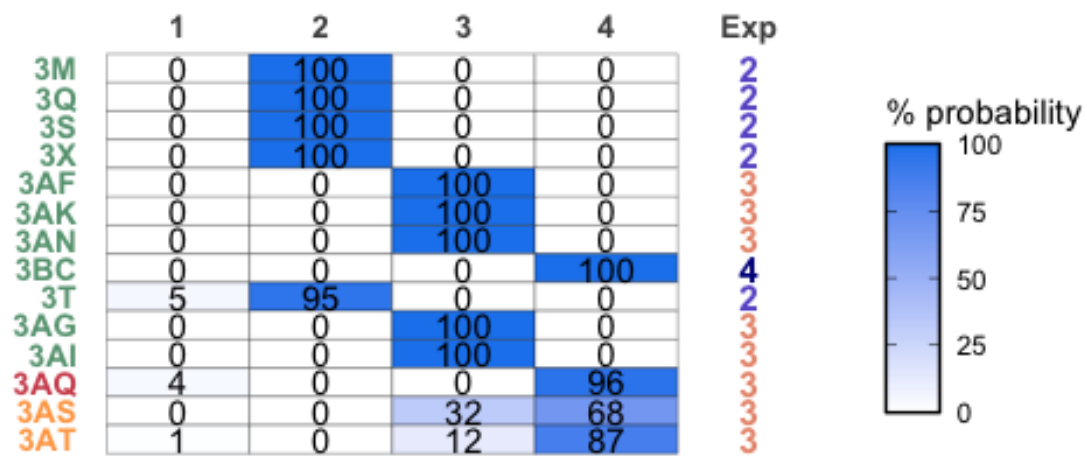
- Accuracy
- False
- Precision
- Size
- True

prop

- 0
- 25
- 50
- 75
- 100

Test Set

Probability Heatmap



10. 10th Place