CH Activation - Model Testing

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formula	McFadden R2
`class ~ fr_NH0 + fr_aldehyde + fr_amide + fr_para_hydroxylation`	0.766
`class ~ fr_Ar_N + fr_aldehyde + fr_amide + fr_para_hydroxylation`	0.764
`class ~ fr_NH0 + fr_aldehyde + fr_amide + fr_pyridine`	0.762
`class ~ fr_aldehyde + fr_amide + fr_para_hydroxylation + fr_pyridine`	0.755
`class ~ fr_Ar_N + fr_NH2 + fr_aldehyde + fr_amide`	0.738
`class ~ fr_C_O + fr_NH0 + fr_NH1 + fr_aldehyde`	0.737
`class ~ fr_C_O_noCOO + fr_NH0 + fr_NH1 + fr_aldehyde`	0.737
`class ~ fr_NH0 + fr_NH1 + fr_aldehyde + fr_amide`	0.737
`class ~ fr_NH0 + fr_NH1 + fr_aldehyde + fr_pyridine`	0.737
`class ~ fr_NH0 + fr_NH2 + fr_aldehyde + fr_amide`	0.737

Section Results Summary

	Training Accuracy	Test Accuracy
1. 1st Place	85.42	83.3
2. 2nd Place	85.42	83.3
3. 3rd Place	85.42	100.0
4. 4th Place	87.50	83.3
5. 5th Place	85.42	83.3
6. 6th Place	83.33	83.3
7. 7th Place	83.33	83.3
8. 8th Place	83.33	83.3
9. 9th Place	83.33	83.3

	Training Accuracy	Test Accuracy
10. 10th Place	83.33	83.3

1st Place

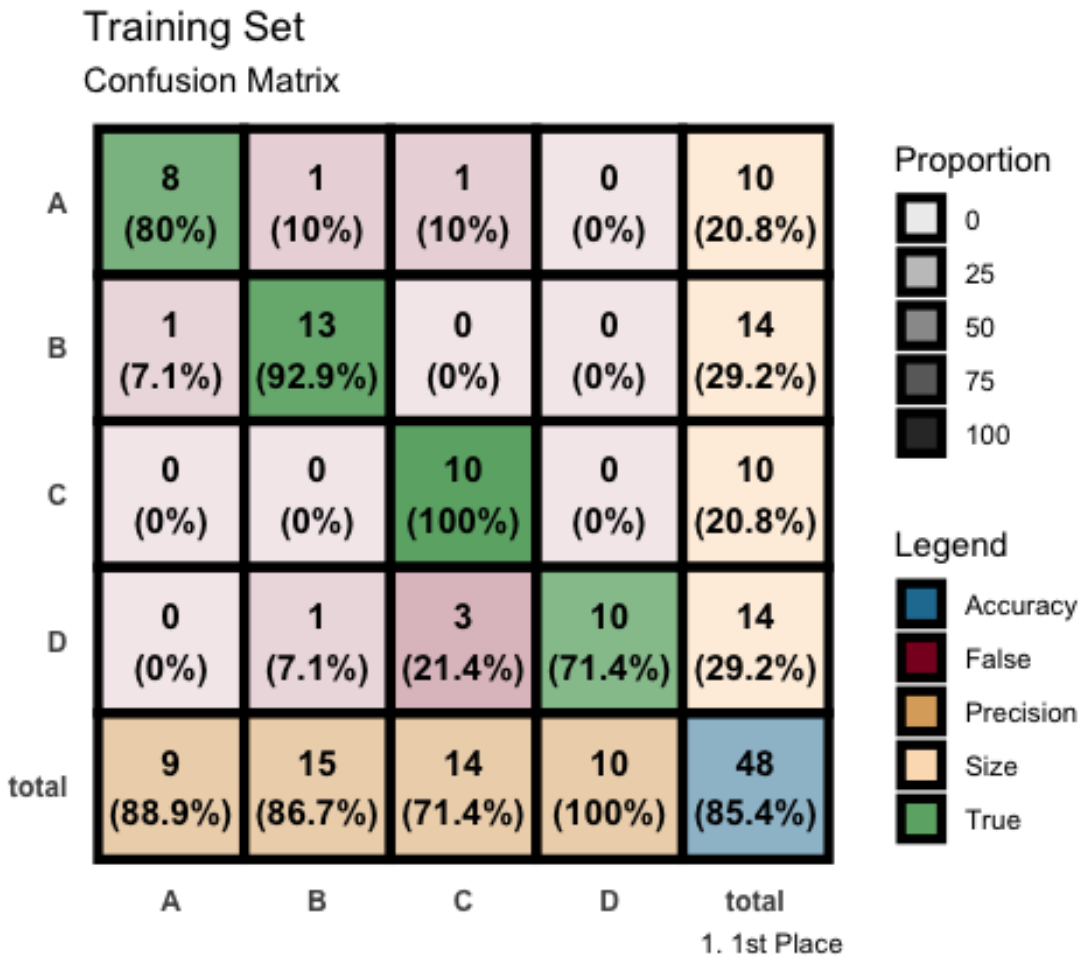
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
85.42%	0.766

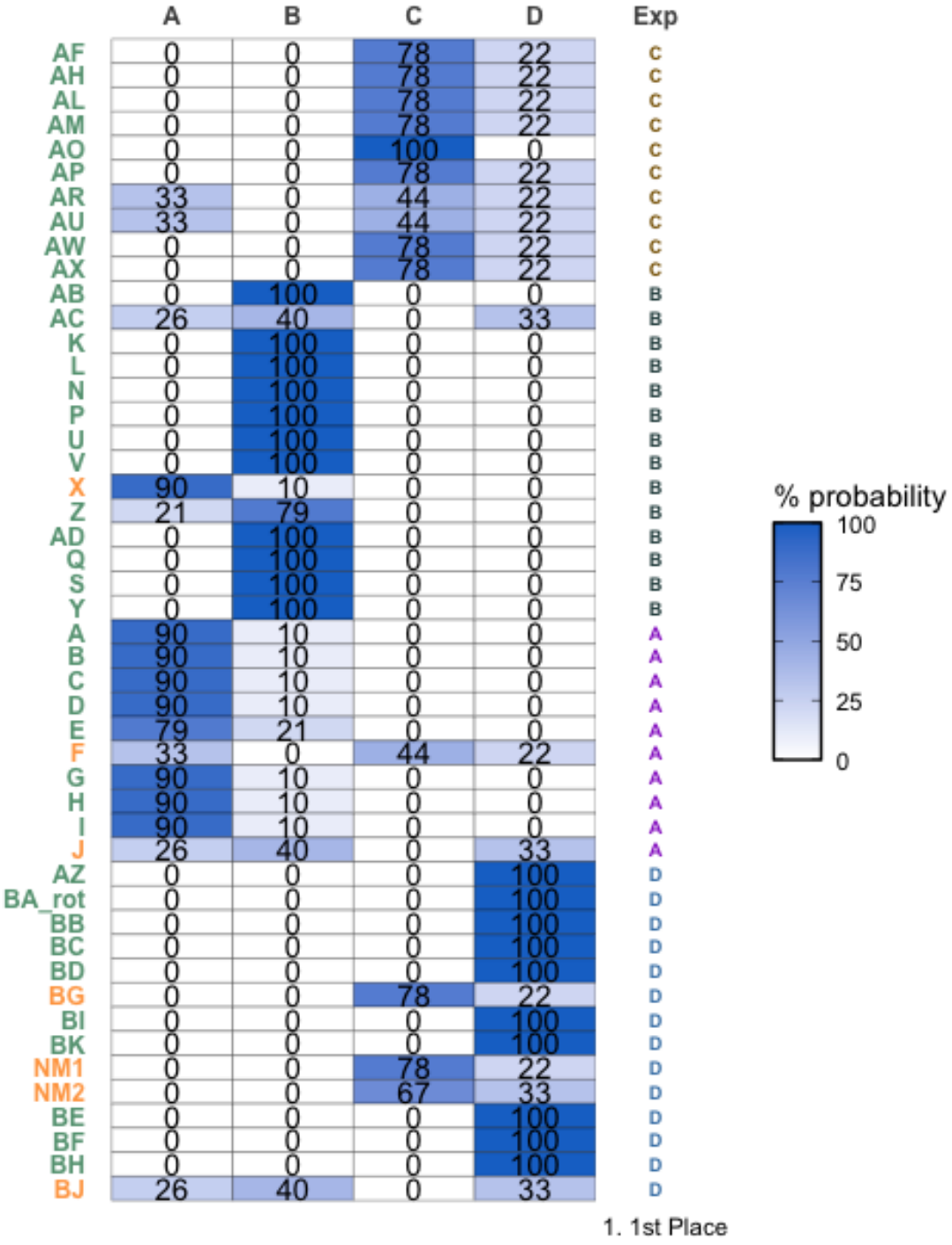
Model Coefficients

	(Intercept)	fr_NH01	fr_NH02	fr_NH05	fr_aldehyde1	fr_amide1	fr_amide2	fr_para_hydroxylation1	fr_para_hydroxylation2
2	89.7468	-91.9592	-89.3189	-11.2499	0.8923468	-52.15421	-15.56946	146.9118	-15.56946
3	32.64020	-205.1309	-59.22859	-4.392311	-205.3117375	172.77838	91.75199	126.8486	91.75199
4	126.42535	-204.5713	-126.18874	31.56324	-220.6162132	77.74052	-60.00557	126.8486	-60.00557

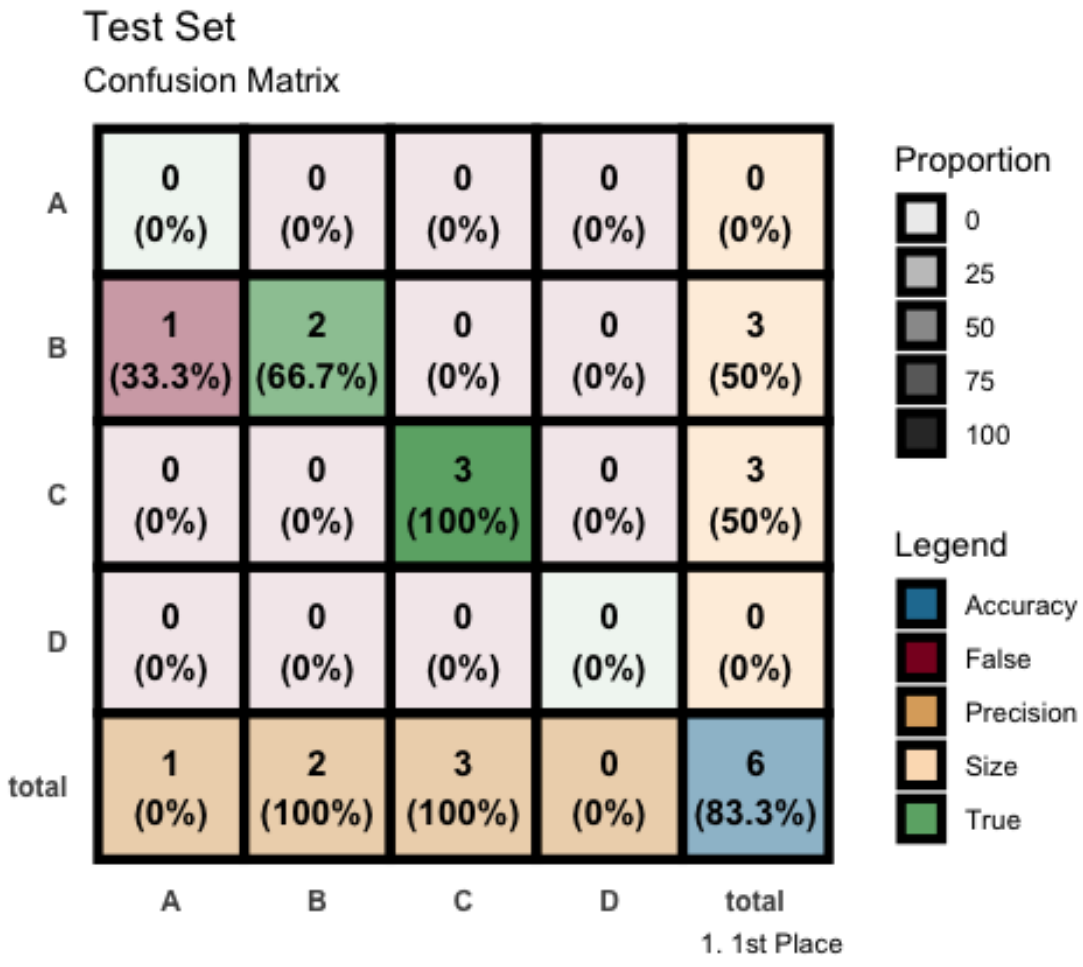

Training Set
Confusion Matrix
A
B
C
D
total
8 (80%)
1 (10%)
1 (10%)
0 (0%)
10 (20.8%)
1 (7.1%)
13 (92.9%)
0 (0%)
0 (0%)
14 (29.2%)
0 (0%)
0 (0%)
10 (100%)
0 (0%)
10 (20.8%)
0 (0%)
1 (7.1%)
3 (21.4%)
10 (71.4%)
14 (29.2%)
9 (88.9%)
15 (86.7%)
14 (71.4%)
10 (100%)
48 (85.4%)
A
B
C
D
total
1. 1st Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Training Set

Probability Heatmap

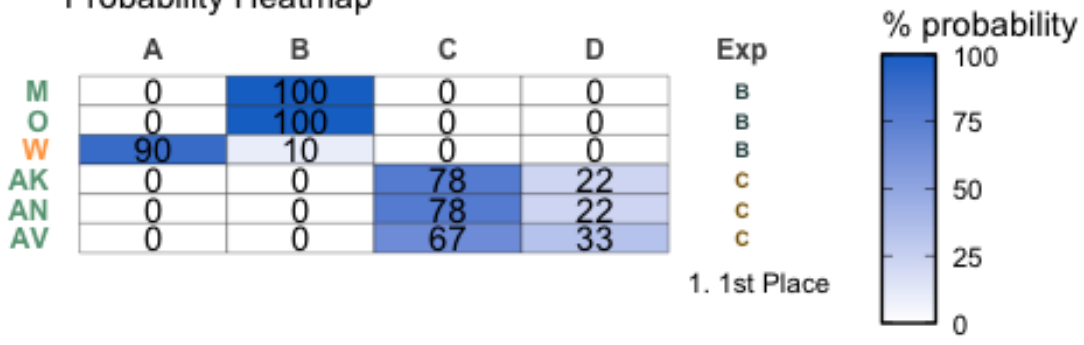


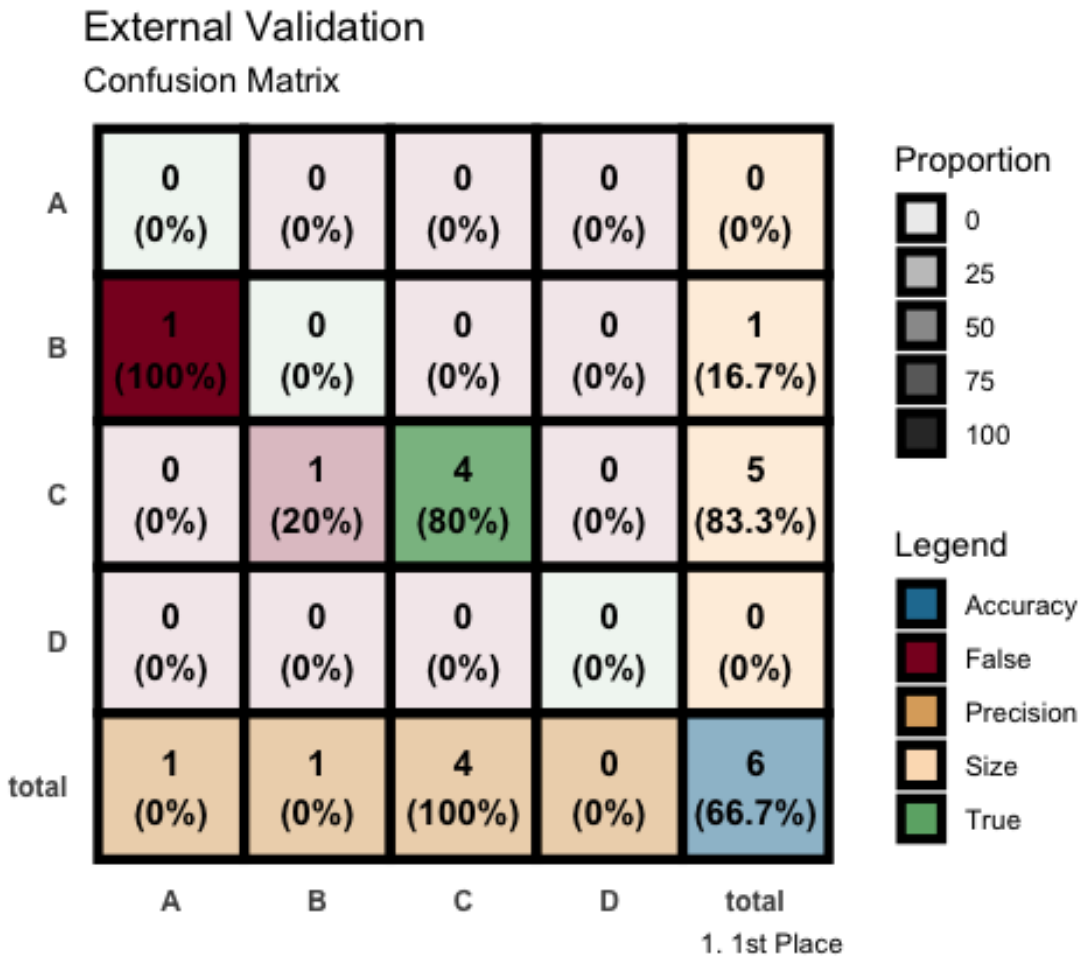
1. 1st Place

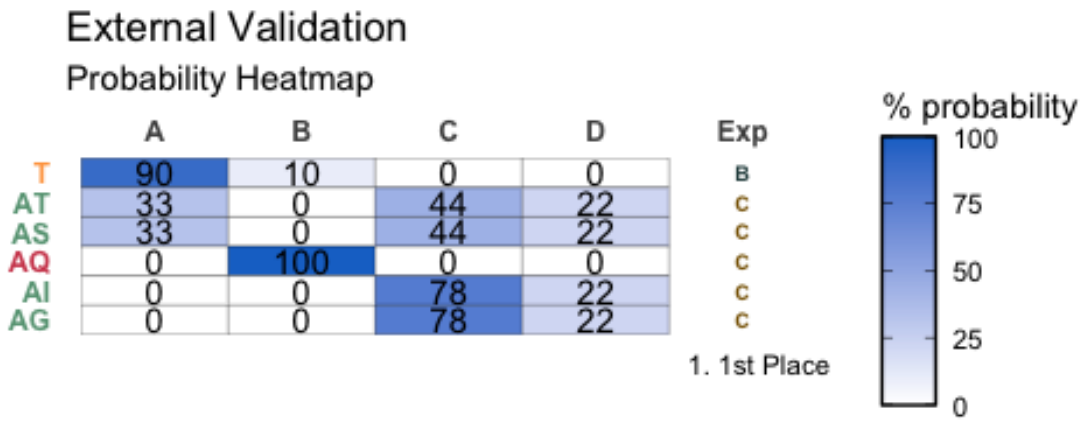

Test Set
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (33.3%)
2 (66.7%)
0 (0%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
2 (100%)
3 (100%)
0 (0%)
6 (83.3%)
A
B
C
D
total
1. 1st Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Test Set

Probability Heatmap




External Validation
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (100%)
0 (0%)
0 (0%)
0 (0%)
1 (16.7%)
0 (0%)
1 (20%)
4 (80%)
0 (0%)
5 (83.3%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
1 (0%)
4 (100%)
0 (0%)
6 (66.7%)
A
B
C
D
total
1. 1st Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True


External Validation
Probability Heatmap
A
B
C
D
Exp
T
AT
AS
AQ
AI
AG
90
10
0
0
B
33
0
44
22
C
33
0
44
22
C
0
100
0
0
C
0
0
78
22
C
0
0
78
22
C
1. 1st Place
% probability
100
75
50
25
0

2nd Place

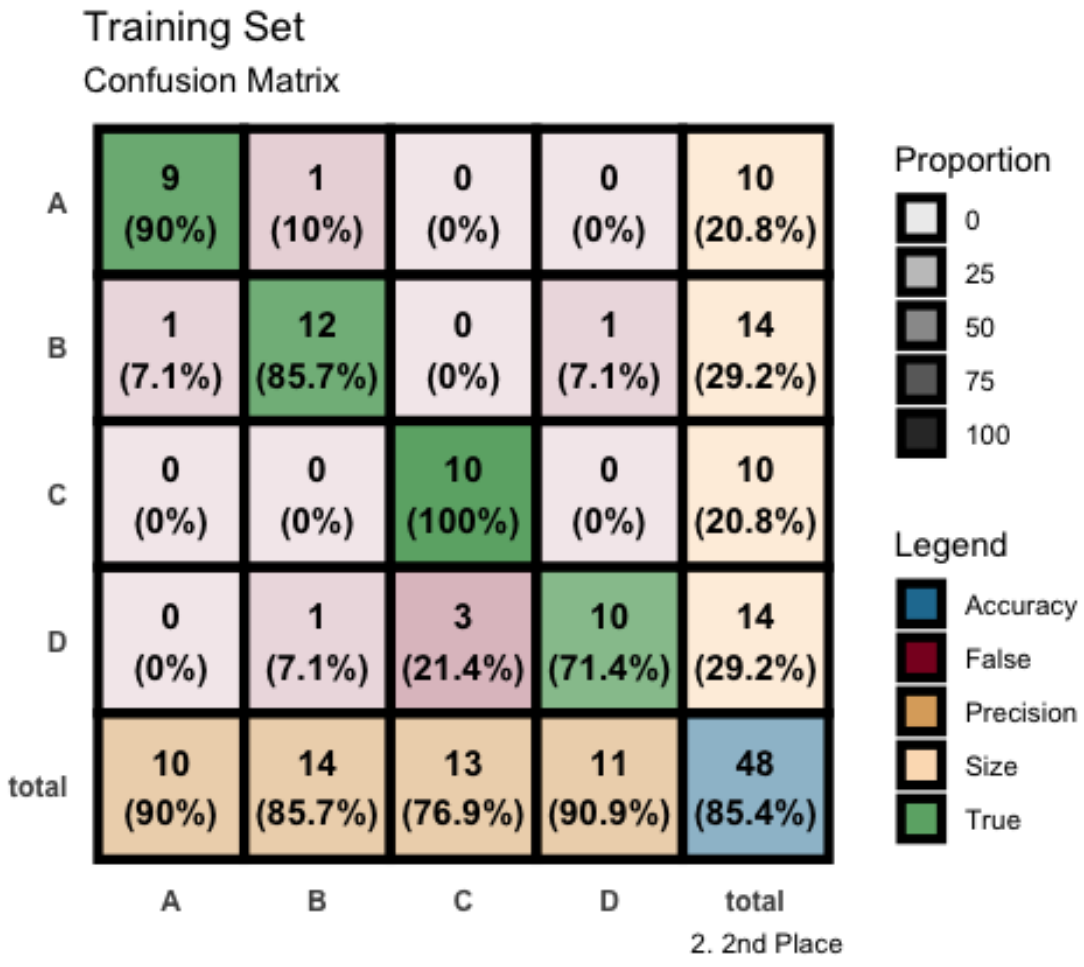
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
85.42%	0.764

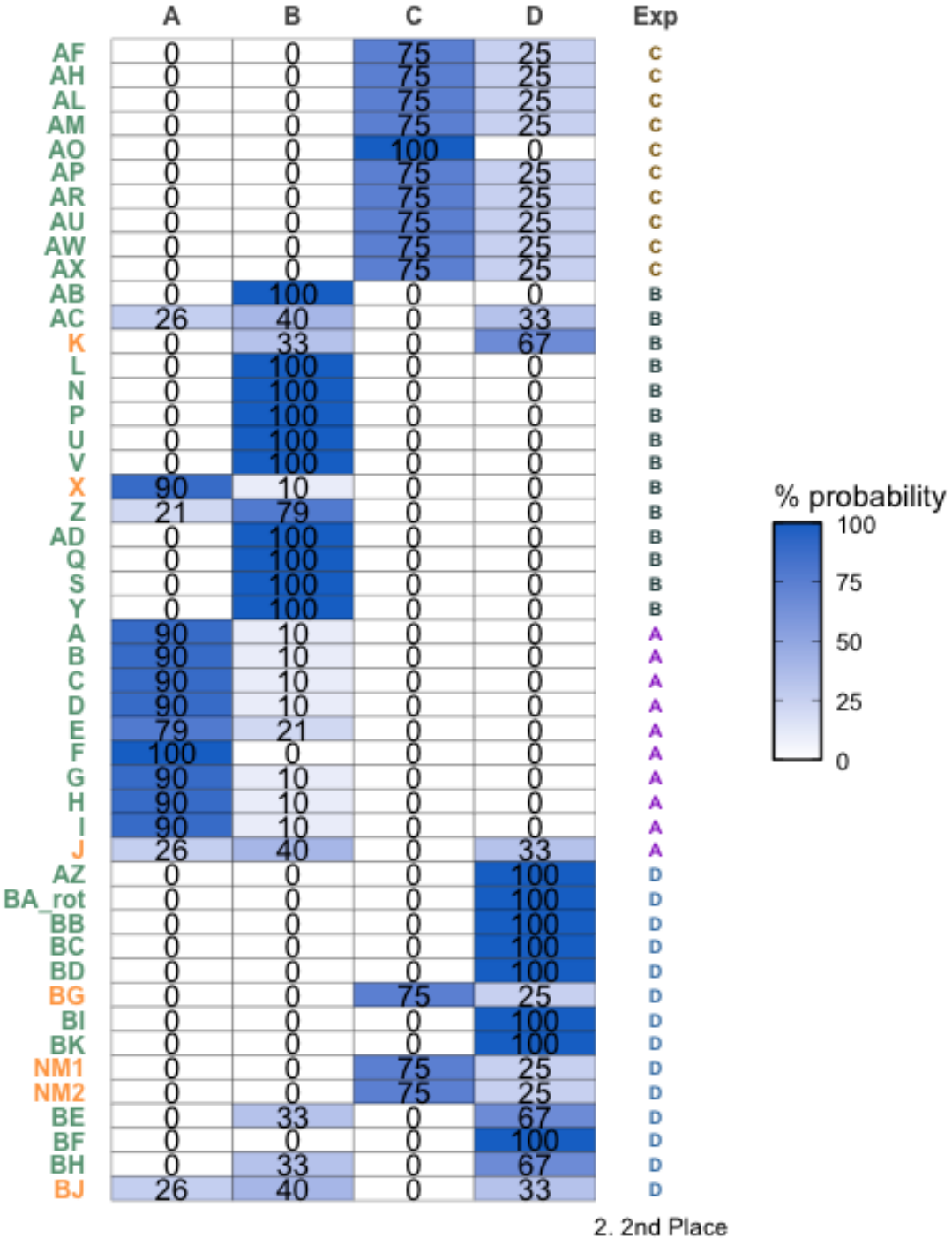
Model Coefficients

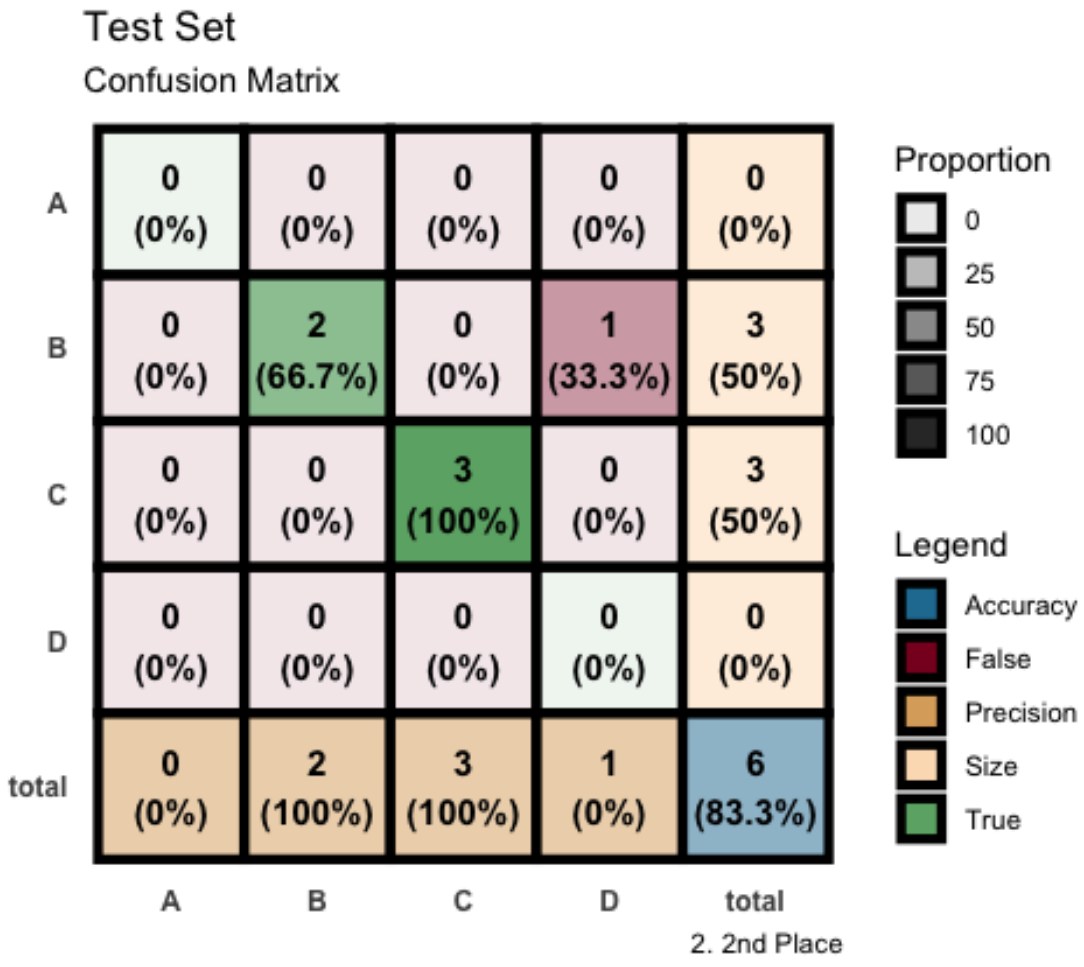
	(Intercept)	fr_Ar_N1	fr_Ar_N2	fr_Ar_N3	fr_aldehyde1	fr_amide1	fr_amide2	fr_para_hydroxylation1	fr_para_hydroxylation2
2	59.70755	-61.91986	-59.27963	-7.165543	0.8922544	-44.348597	-9.332006	73.95221	-9.332006
3	12.76279	-156.77406	-45.23150	-2.129974	-102.9557782	72.556856	55.071413	51.74269	55.071413
4	82.61025	-125.29993	-82.37361	17.942911	-117.5485908	1.610791	-31.509658	51.74267	-31.509658


Training Set
Confusion Matrix
A
B
C
D
total
9 (90%)
1 (10%)
0 (0%)
0 (0%)
10 (20.8%)
1 (7.1%)
12 (85.7%)
0 (0%)
1 (7.1%)
14 (29.2%)
0 (0%)
0 (0%)
10 (100%)
0 (0%)
10 (20.8%)
0 (0%)
1 (7.1%)
3 (21.4%)
10 (71.4%)
14 (29.2%)
10 (90%)
14 (85.7%)
13 (76.9%)
11 (90.9%)
48 (85.4%)
A
B
C
D
total
2. 2nd Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Training Set

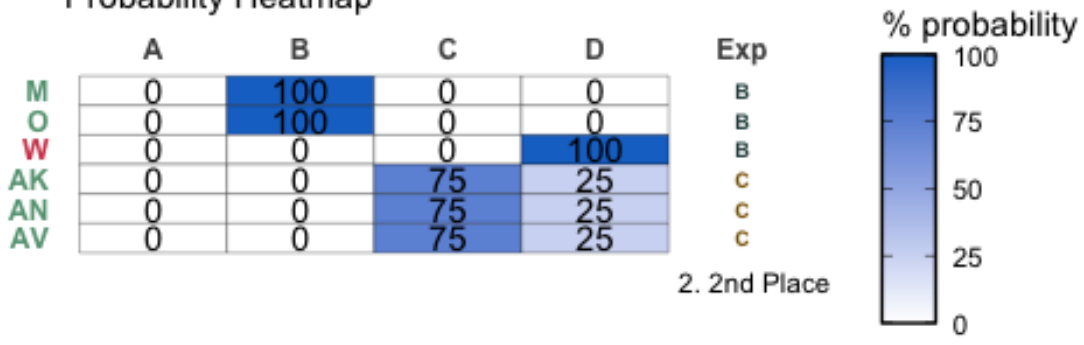
Probability Heatmap

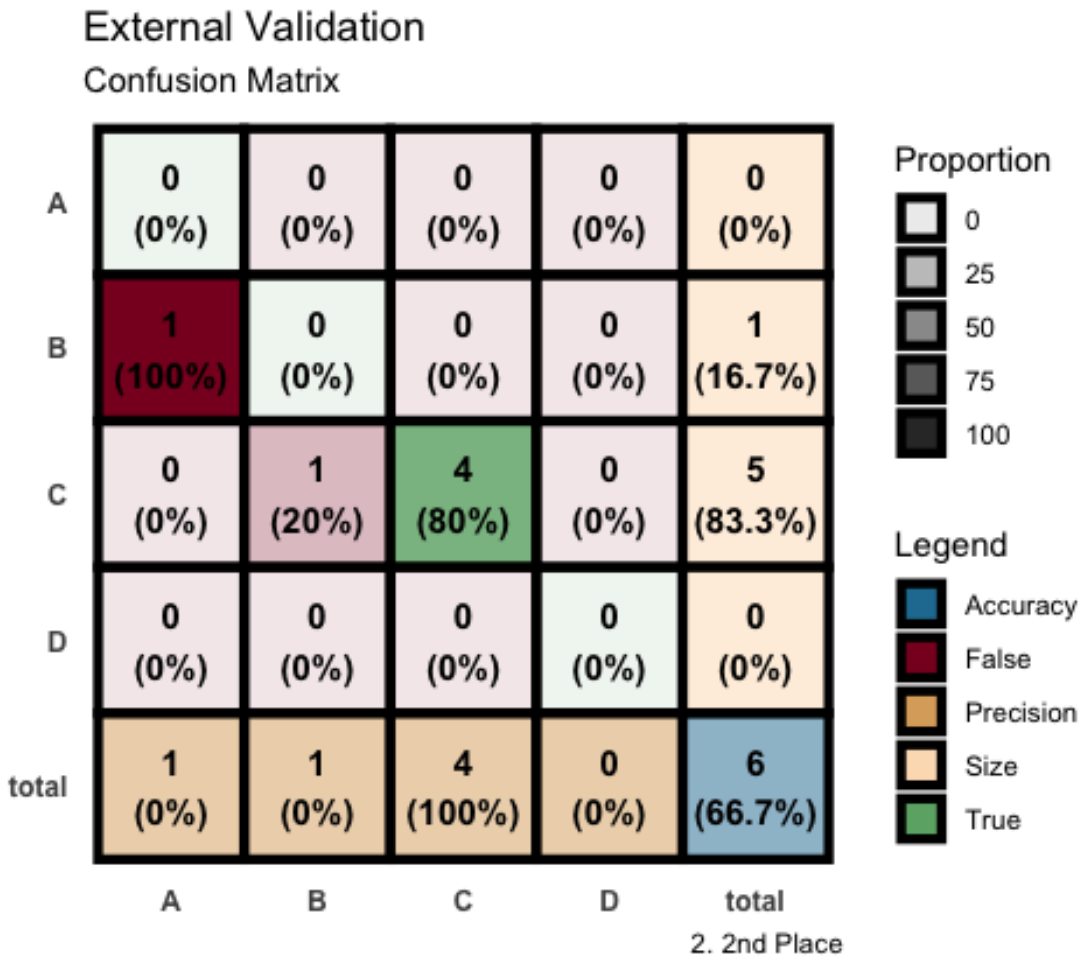



Test Set
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
2 (66.7%)
0 (0%)
1 (33.3%)
3 (50%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
2 (100%)
3 (100%)
1 (0%)
6 (83.3%)
A
B
C
D
total
2. 2nd Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Test Set

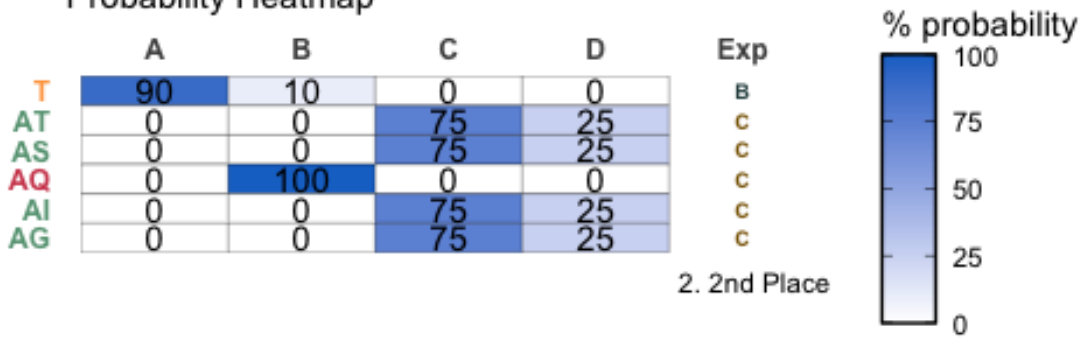
Probability Heatmap




External Validation
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (100%)
0 (0%)
0 (0%)
0 (0%)
1 (16.7%)
0 (0%)
1 (20%)
4 (80%)
0 (0%)
5 (83.3%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
1 (0%)
4 (100%)
0 (0%)
6 (66.7%)
A
B
C
D
total
2. 2nd Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

External Validation

Probability Heatmap



3rd Place

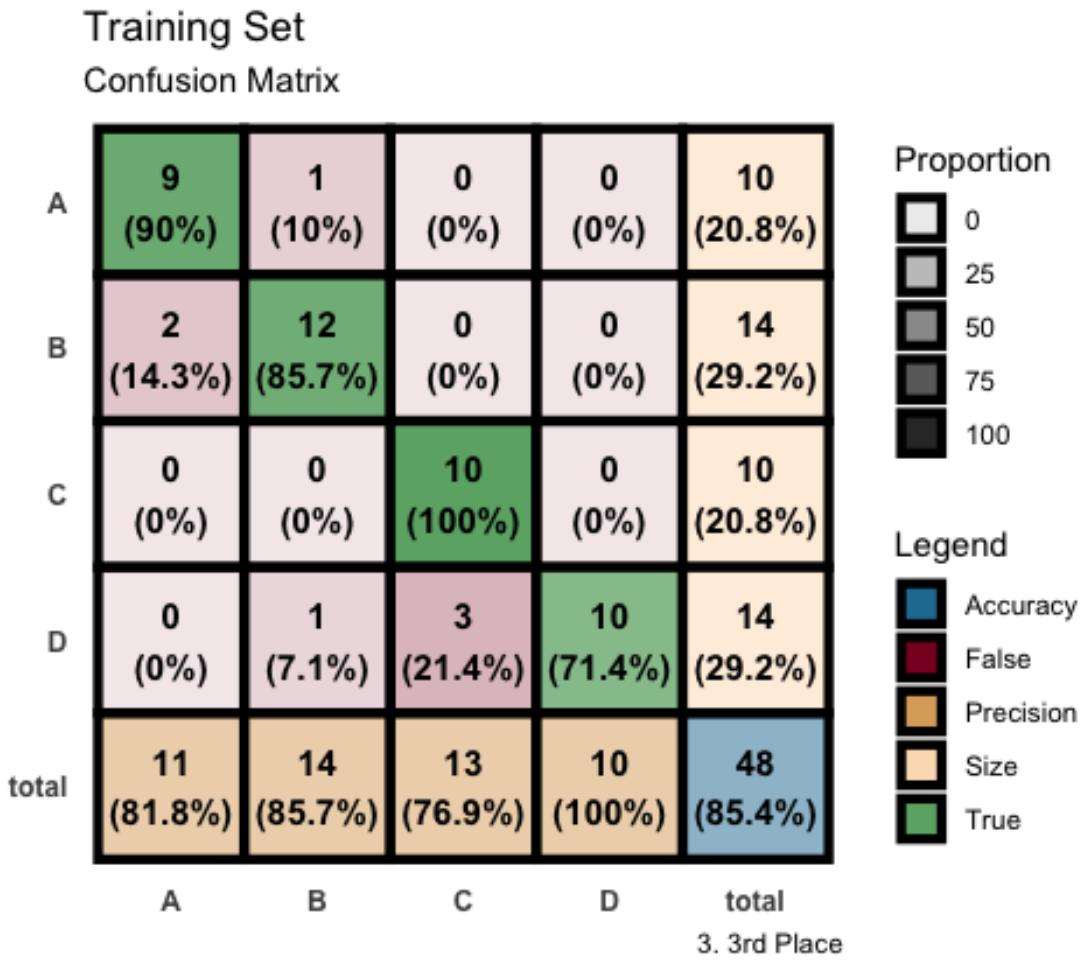
Table:

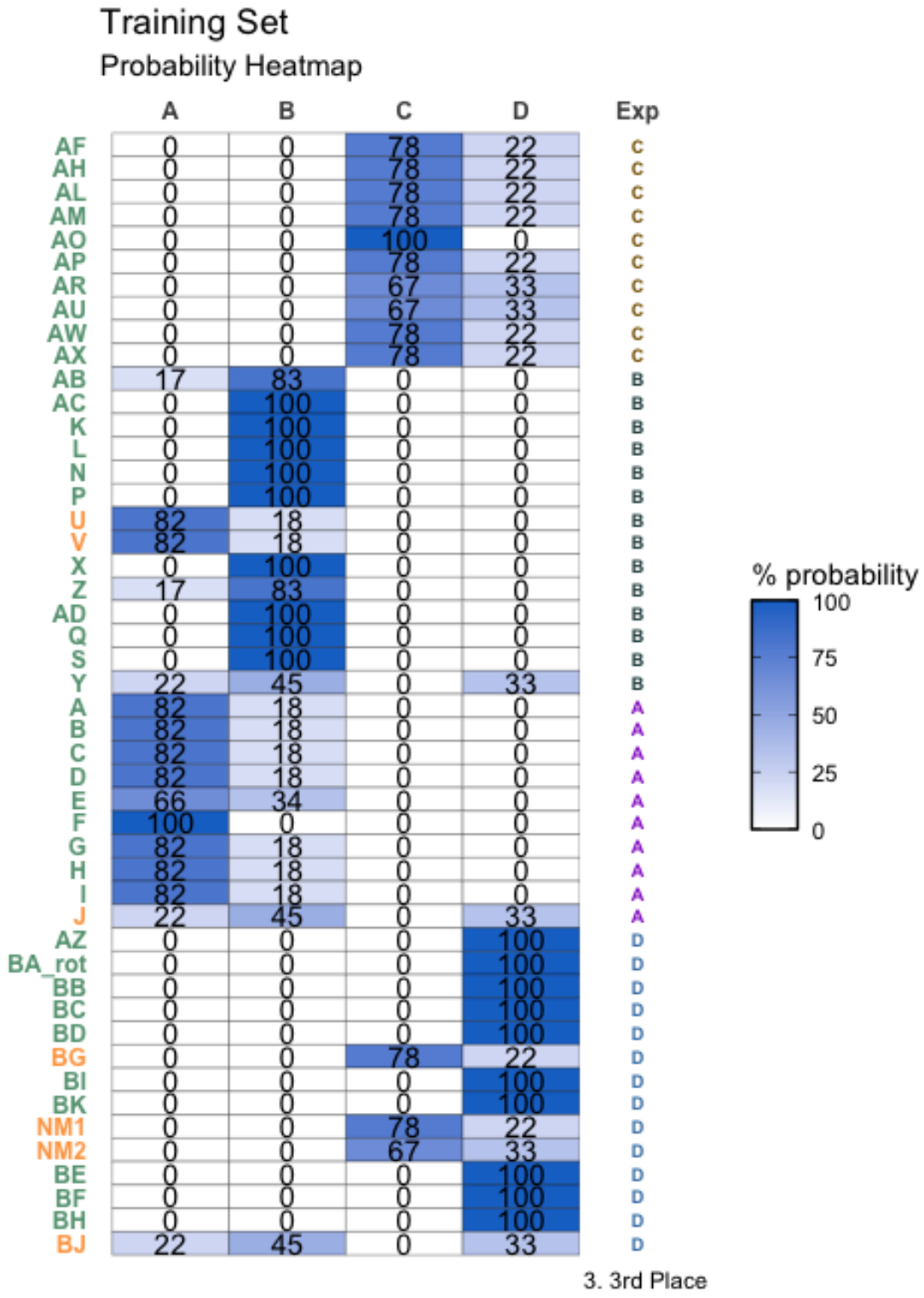
Full Model Stats - Overall Accuracy and Pseudo-R2

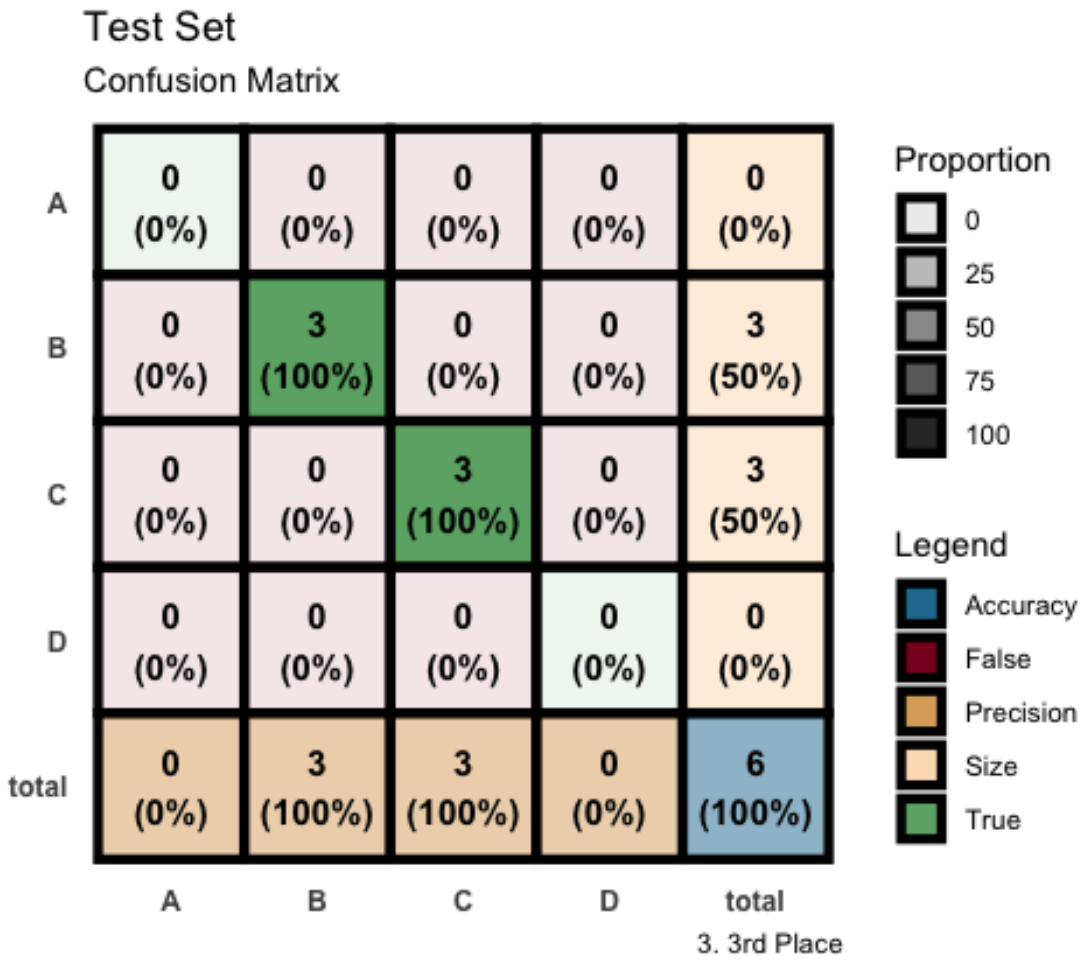
Accuracy	McFadden_R2
85.42%	0.762

Model Coefficients

	(Intercept)	fr_NH01	fr_NH02	fr_NH05	fr_aldehyde1	fr_amide1	fr_amide2	fr_pyridine1	fr_pyridine2
2	77.146276	7.613779	-76.42688	-11.946103	0.8488433	-56.07204	-20.52782	-86.25024	78.008171
3	8.319367	-52.025492	-57.35079	-3.910005	-185.0473453	103.38214	111.78747	-162.83443	-3.618838
4	95.677264	-51.465887	-95.25421	24.534540	-196.7872443	14.77146	-72.36790	-155.40107	-33.275126

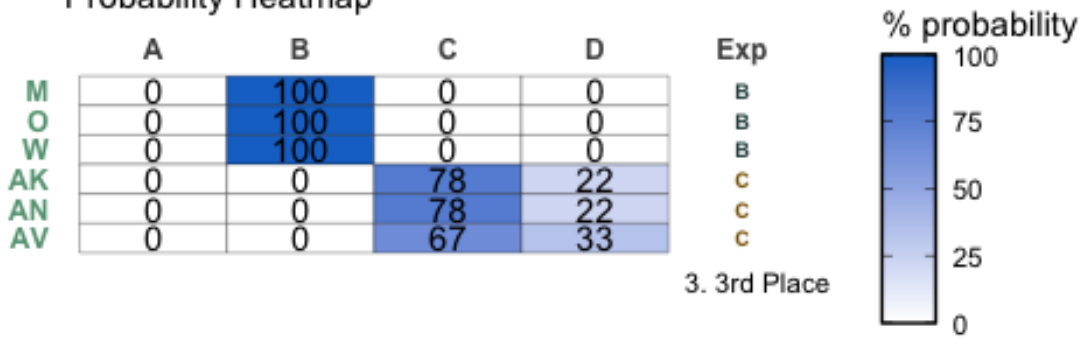

Training Set
Confusion Matrix
A
B
C
D
total
9 (90%)
1 (10%)
0 (0%)
0 (0%)
10 (20.8%)
2 (14.3%)
12 (85.7%)
0 (0%)
0 (0%)
14 (29.2%)
0 (0%)
0 (0%)
10 (100%)
0 (0%)
10 (20.8%)
0 (0%)
1 (7.1%)
3 (21.4%)
10 (71.4%)
14 (29.2%)
11 (81.8%)
14 (85.7%)
13 (76.9%)
10 (100%)
48 (85.4%)
A
B
C
D
total
3. 3rd Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

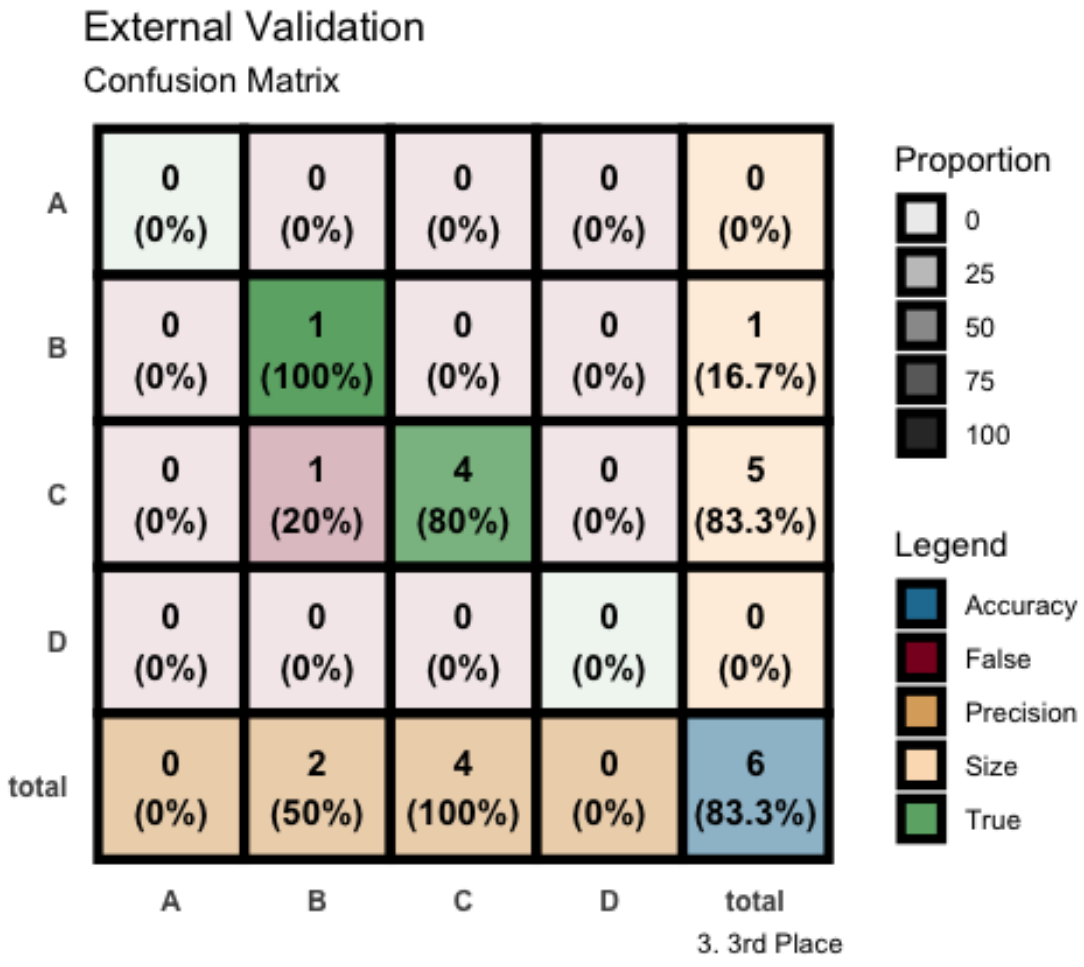

Training Set
Probability Heatmap
A
B
C
D
Exp
AF 0 0 78 22 C
AH 0 0 78 22 C
AL 0 0 78 22 C
AM 0 0 78 22 C
AO 0 0 100 0 C
AP 0 0 78 22 C
AR 0 0 67 33 C
AU 0 0 67 33 C
AW 0 0 78 22 C
AX 0 0 78 22 C
AB 17 83 0 0 B
AC 0 100 0 0 B
K 0 100 0 0 B
L 0 100 0 0 B
N 0 100 0 0 B
P 0 100 0 0 B
U 82 18 0 0 B
V 82 18 0 0 B
X 0 100 0 0 B
Z 17 83 0 0 B
AD 0 100 0 0 B
Q 0 100 0 0 B
S 0 100 0 0 B
Y 22 45 0 33 B
A 82 18 0 0 A
B 82 18 0 0 A
C 82 18 0 0 A
D 82 18 0 0 A
E 66 34 0 0 A
F 100 0 0 0 A
G 82 18 0 0 A
H 82 18 0 0 A
I 82 18 0 0 A
J 22 45 0 33 A
AZ 0 0 0 100 D
BA_rot 0 0 0 100 D
BB 0 0 0 100 D
BC 0 0 0 100 D
BD 0 0 0 100 D
BG 0 0 78 22 D
BI 0 0 0 100 D
BK 0 0 0 100 D
NM1 0 0 78 22 D
NM2 0 0 67 33 D
BE 0 0 0 100 D
BF 0 0 0 100 D
BH 0 0 0 100 D
BJ 22 45 0 33 D
% probability
100
75
50
25
0
3. 3rd Place


Test Set
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
3 (100%)
3 (100%)
0 (0%)
6 (100%)
A
B
C
D
total
3. 3rd Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Test Set

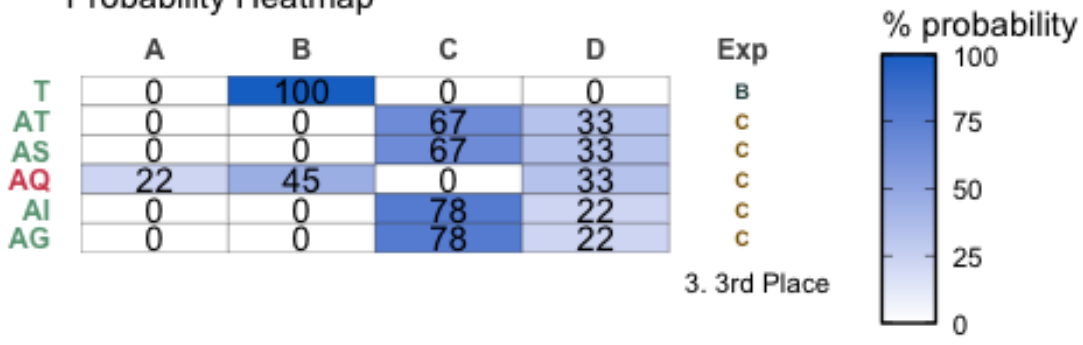
Probability Heatmap




External Validation
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (100%)
0 (0%)
0 (0%)
1 (16.7%)
0 (0%)
1 (20%)
4 (80%)
0 (0%)
5 (83.3%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
2 (50%)
4 (100%)
0 (0%)
6 (83.3%)
A
B
C
D
total
3. 3rd Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

External Validation

Probability Heatmap



4th Place

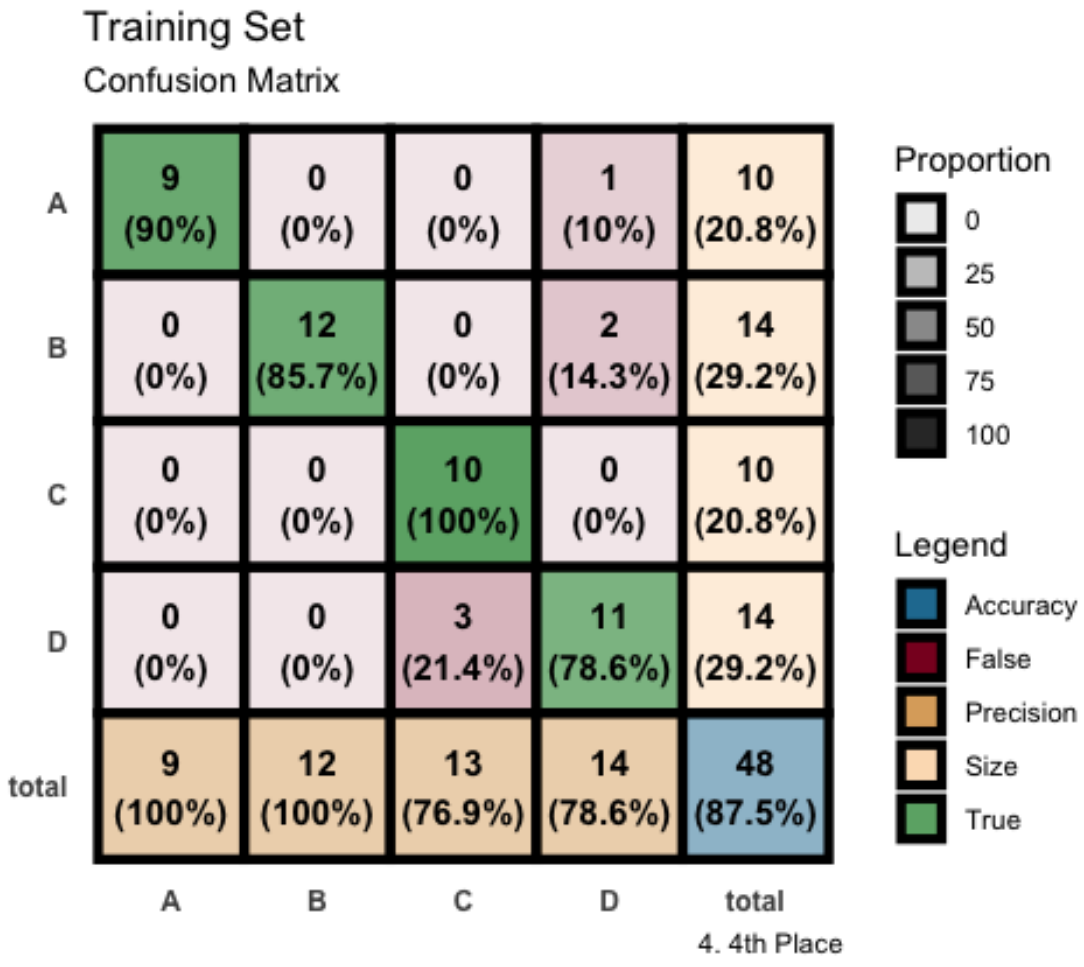
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
87.5%	0.755

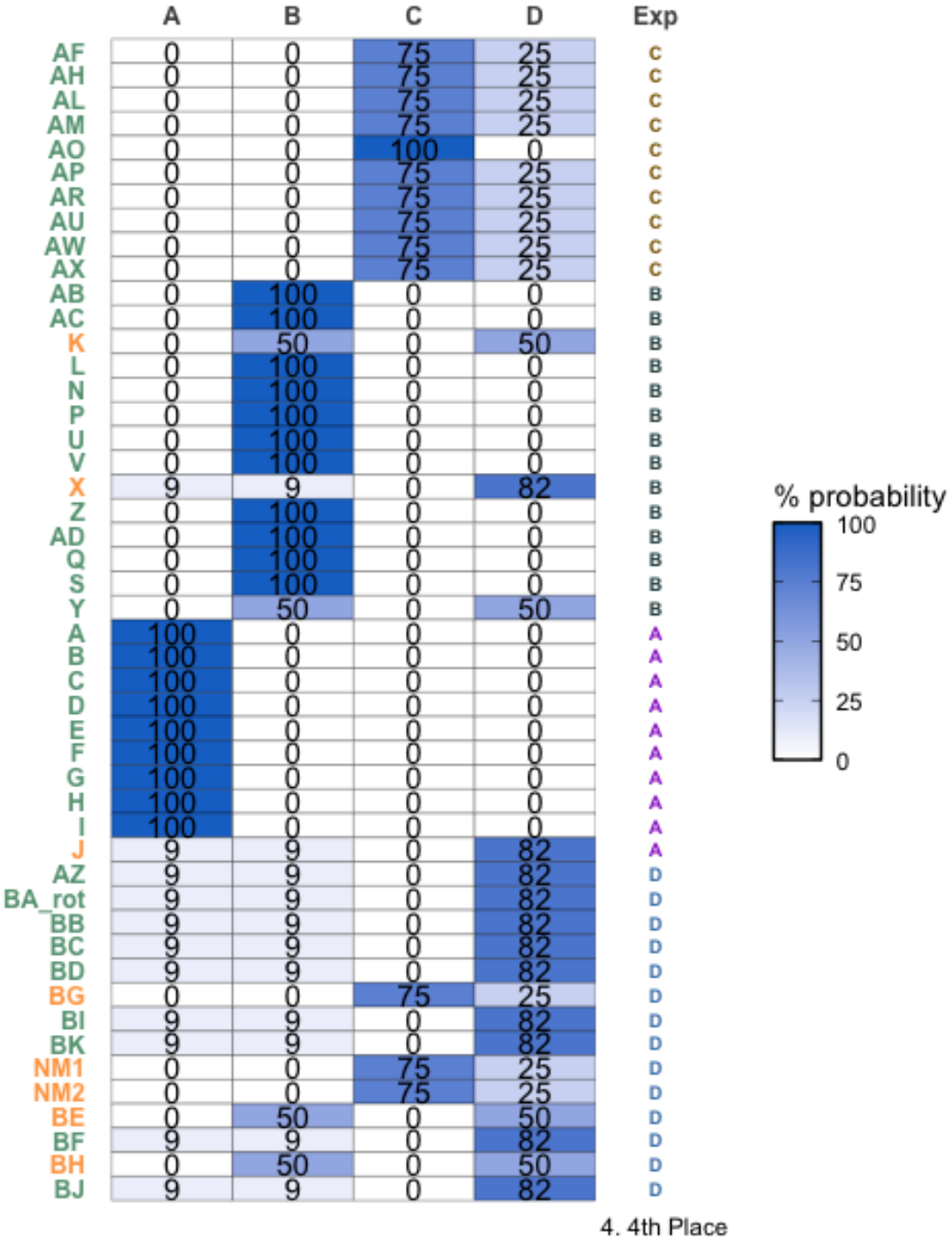
Model Coefficients

	(Intercept)	fr_aldehyde1	fr_amide1	fr_amide2	fr_para_hydroxylation1	fr_para_hydroxylation2	fr_pyridine1	fr_pyridine2
2	0.0000181	29.46578	14.76031	-11.69553	116.6129	-11.69553	-64.06825	71.87472
3	-16.3206609	-66.19000	73.79567	61.55836	114.4155	61.55836	-90.04795	-2.90876
4	2.1972931	-56.25133	54.17908	-30.82048	114.4156	-30.82048	-104.88701	-46.90315

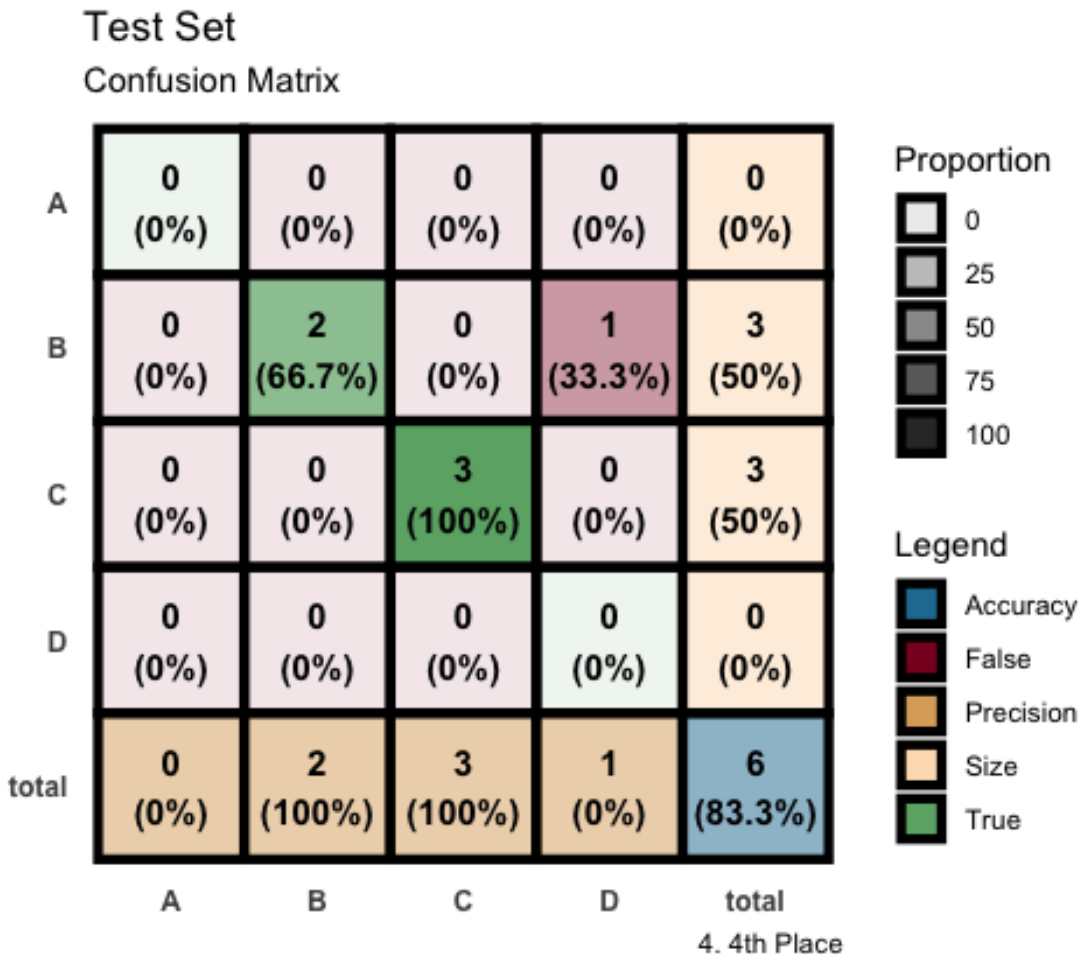

Training Set
Confusion Matrix
A
B
C
D
total
9 (90%)
0 (0%)
0 (0%)
1 (10%)
10 (20.8%)
0 (0%)
12 (85.7%)
0 (0%)
2 (14.3%)
14 (29.2%)
0 (0%)
0 (0%)
10 (100%)
0 (0%)
10 (20.8%)
0 (0%)
0 (0%)
3 (21.4%)
11 (78.6%)
14 (29.2%)
9 (100%)
12 (100%)
13 (76.9%)
14 (78.6%)
48 (87.5%)
A
B
C
D
total
4. 4th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Training Set

Probability Heatmap

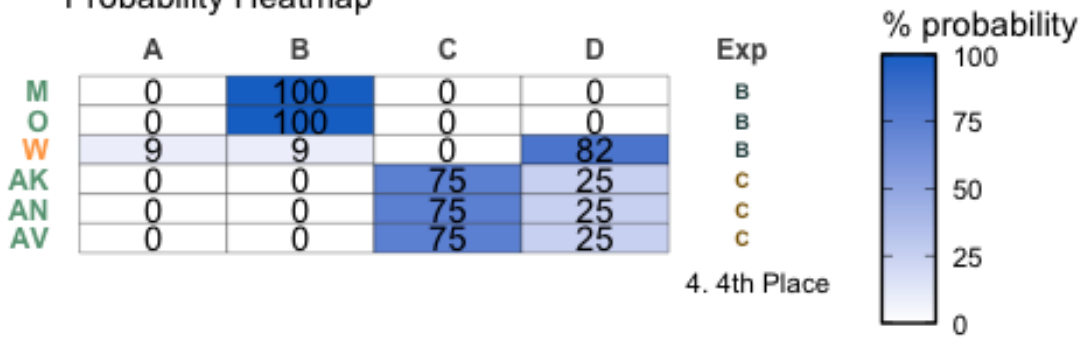


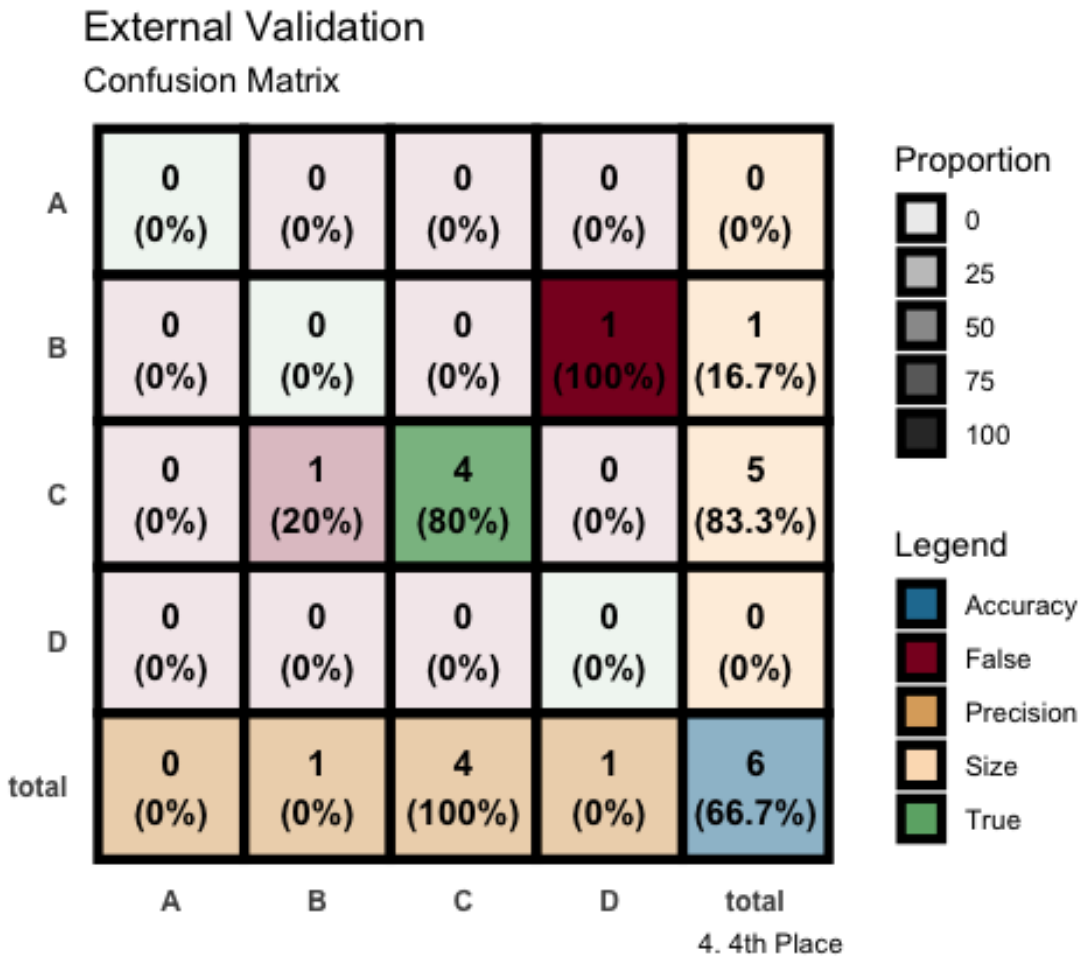
4. 4th Place


Test Set
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
2 (66.7%)
0 (0%)
1 (33.3%)
3 (50%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
2 (100%)
3 (100%)
1 (0%)
6 (83.3%)
A
B
C
D
total
4. 4th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Test Set

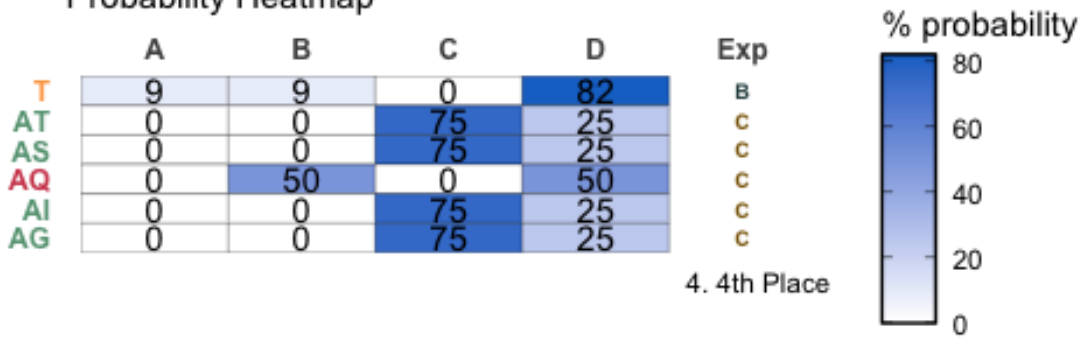
Probability Heatmap




External Validation
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (100%)
1 (16.7%)
0 (0%)
1 (20%)
4 (80%)
0 (0%)
5 (83.3%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
4 (100%)
1 (0%)
6 (66.7%)
A
B
C
D
total
4. 4th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

External Validation

Probability Heatmap



5th Place

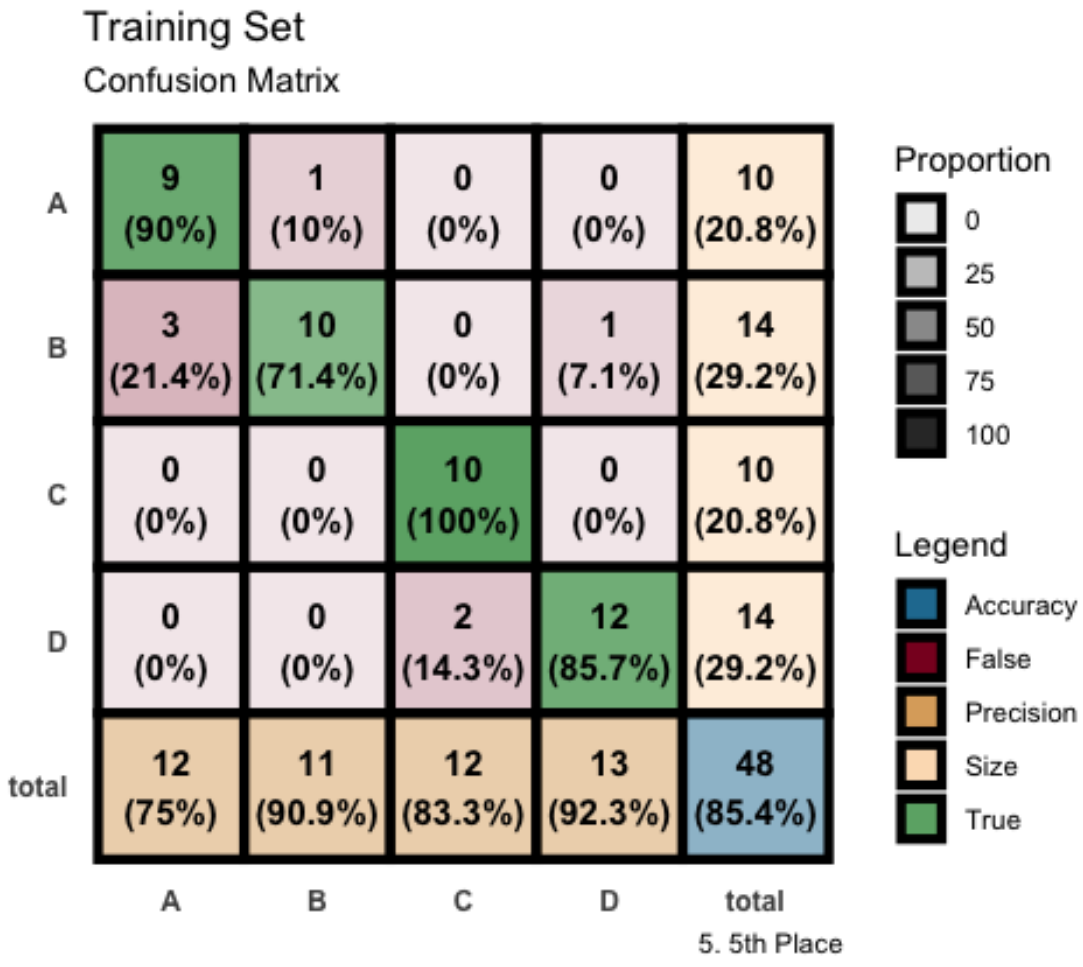
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
85.42%	0.738

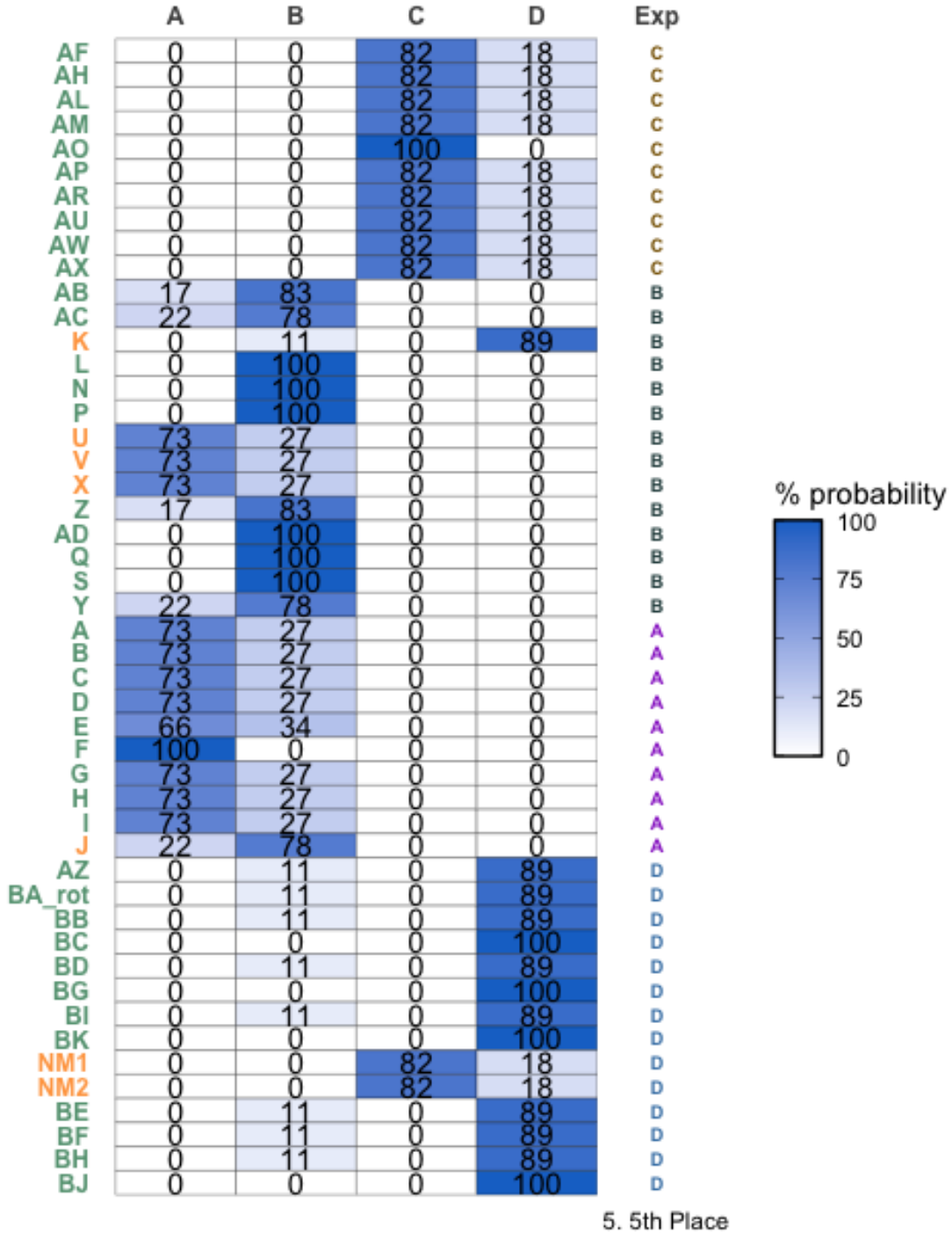
Model Coefficients

	(Intercept)	fr_Ar_N1	fr_Ar_N2	fr_Ar_N3	fr_NH21	fr_aldehyde1	fr_amide1	fr_amide2
2	59.850481	-60.86394	-58.59069	-9.573486	-20.00759	0.3366145	-36.04984	-13.01705
3	8.976537	-77.20032	-25.85147	-2.184739	-13.53670	-59.392328	52.05684	73.38108
4	61.929923	-87.74431	-85.87365	20.718103	52.72304	-69.533214	-2.400612	-42.89410

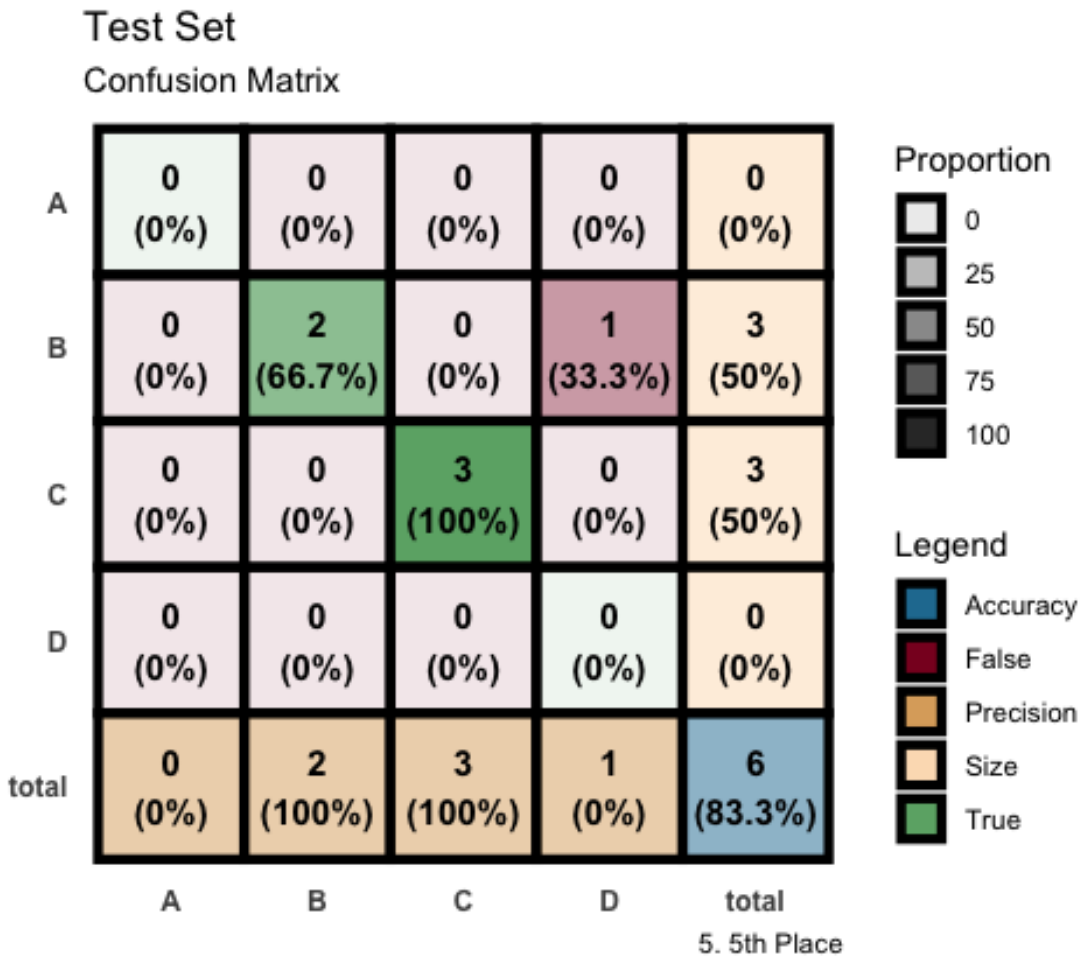

Training Set
Confusion Matrix
A
B
C
D
total
9 (90%)
1 (10%)
0 (0%)
0 (0%)
10 (20.8%)
3 (21.4%)
10 (71.4%)
0 (0%)
1 (7.1%)
14 (29.2%)
0 (0%)
0 (0%)
10 (100%)
0 (0%)
10 (20.8%)
0 (0%)
0 (0%)
2 (14.3%)
12 (85.7%)
14 (29.2%)
12 (75%)
11 (90.9%)
12 (83.3%)
13 (92.3%)
48 (85.4%)
A
B
C
D
total
5. 5th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Training Set

Probability Heatmap

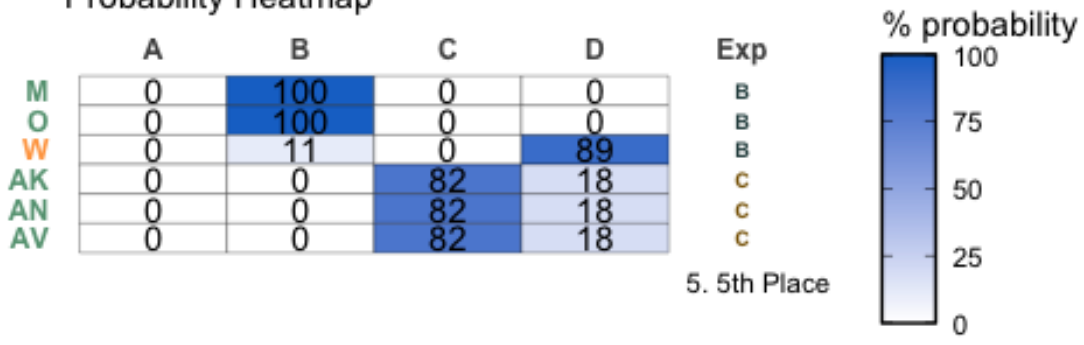


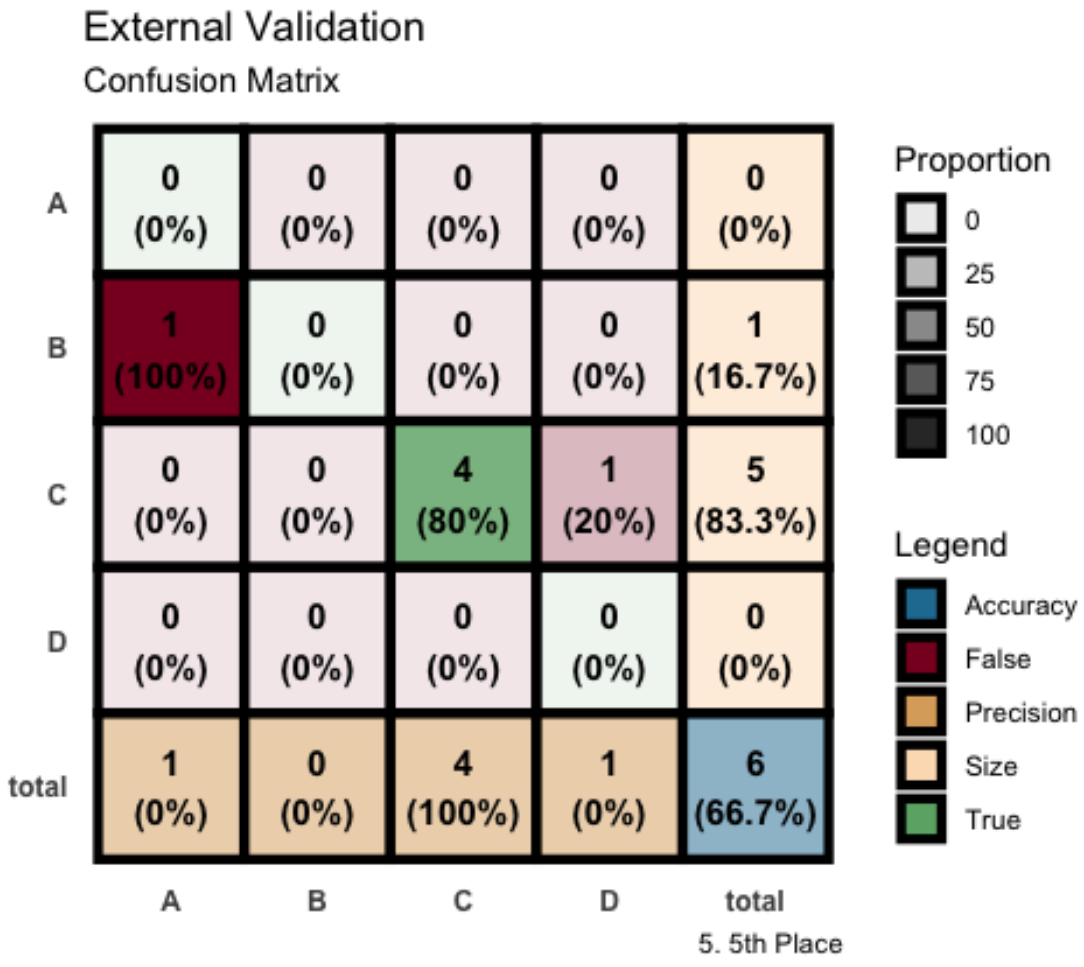
5. 5th Place


Test Set
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
2 (66.7%)
0 (0%)
1 (33.3%)
3 (50%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
2 (100%)
3 (100%)
1 (0%)
6 (83.3%)
A
B
C
D
total
5. 5th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Test Set

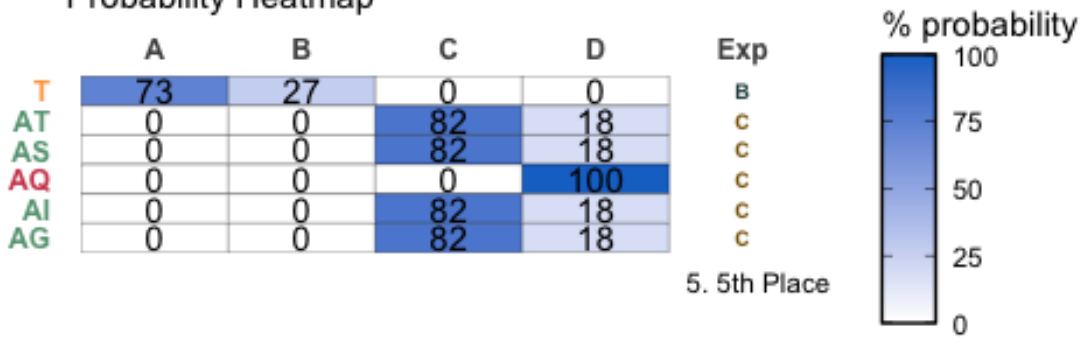
Probability Heatmap




External Validation
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (100%)
0 (0%)
0 (0%)
0 (0%)
1 (16.7%)
0 (0%)
0 (0%)
4 (80%)
1 (20%)
5 (83.3%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
0 (0%)
4 (100%)
1 (0%)
6 (66.7%)
A
B
C
D
total
5. 5th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

External Validation

Probability Heatmap



6th Place

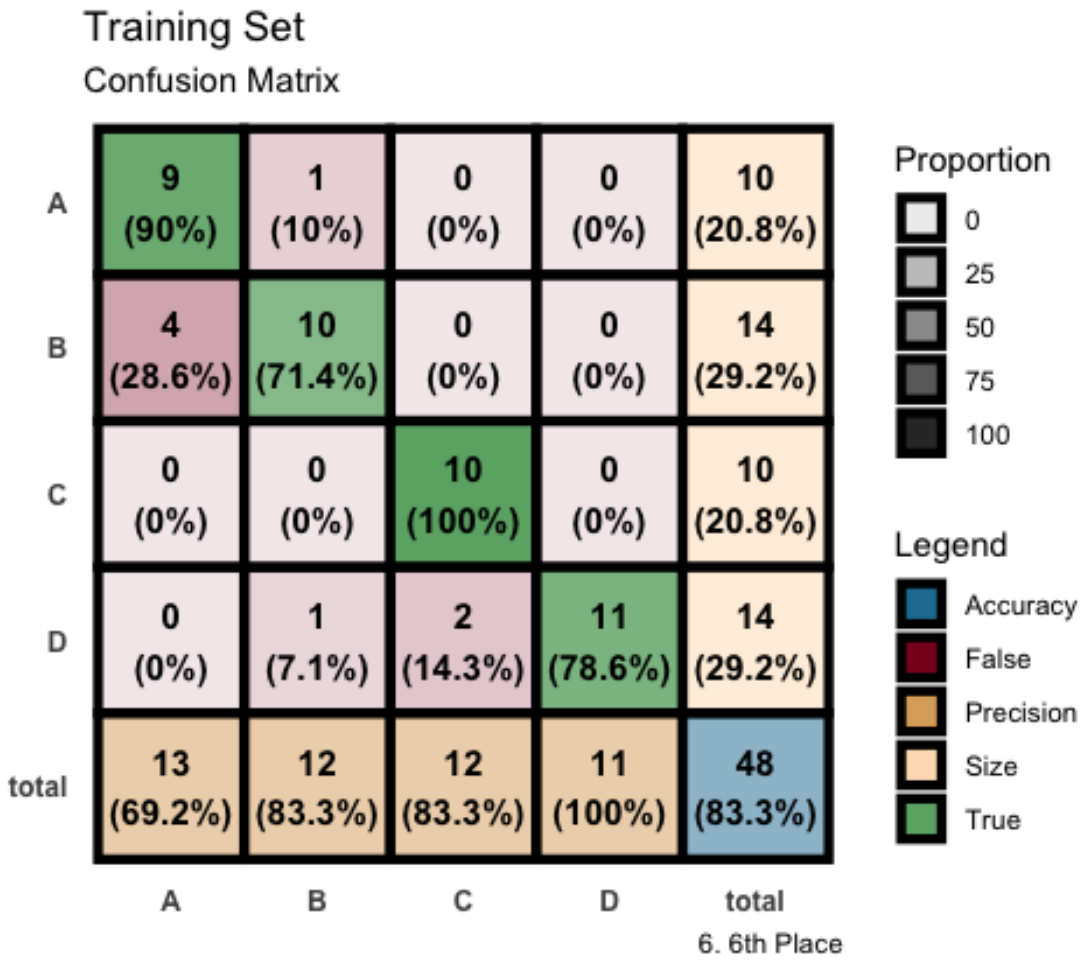
Table:

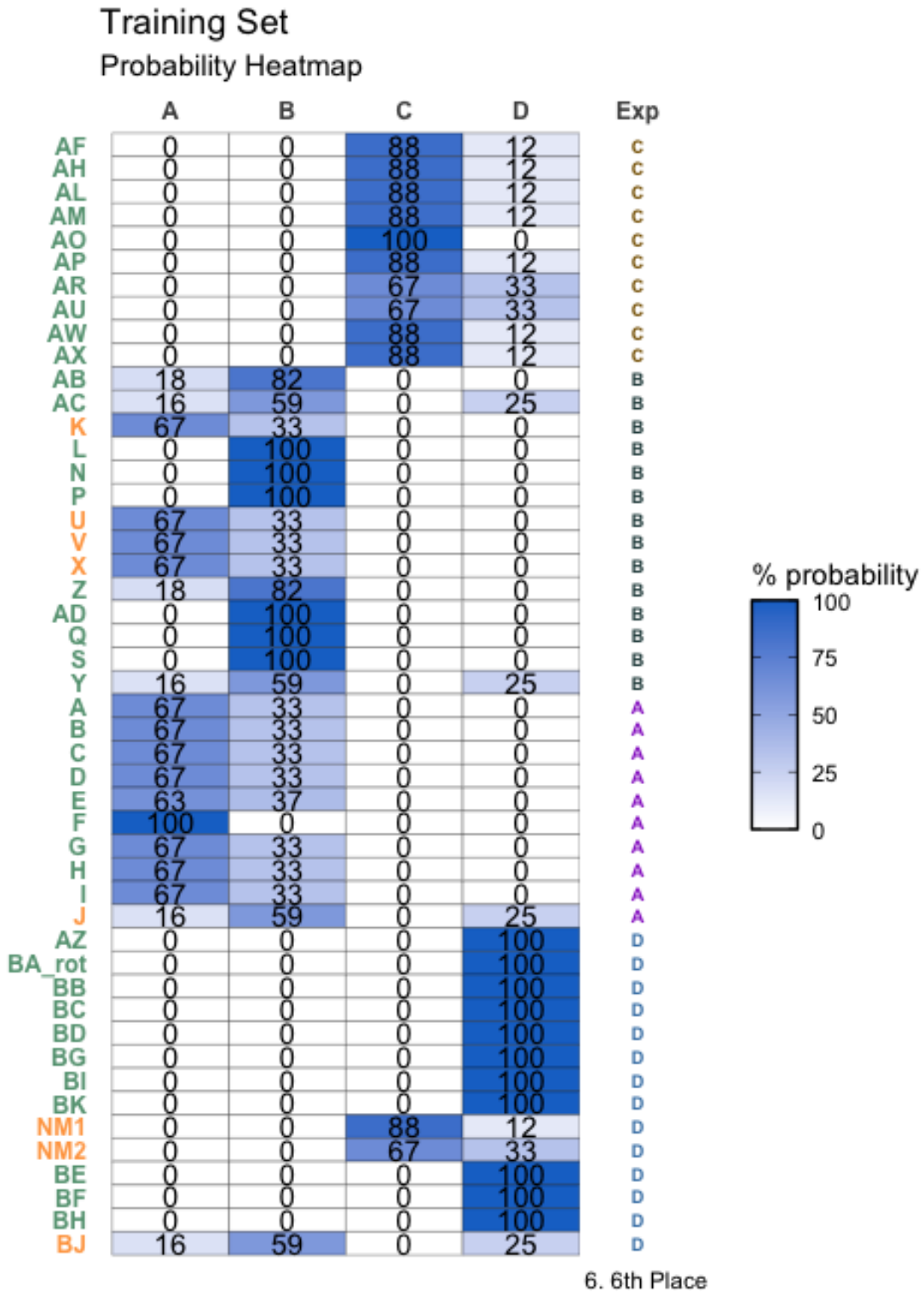
Full Model Stats - Overall Accuracy and Pseudo-R2

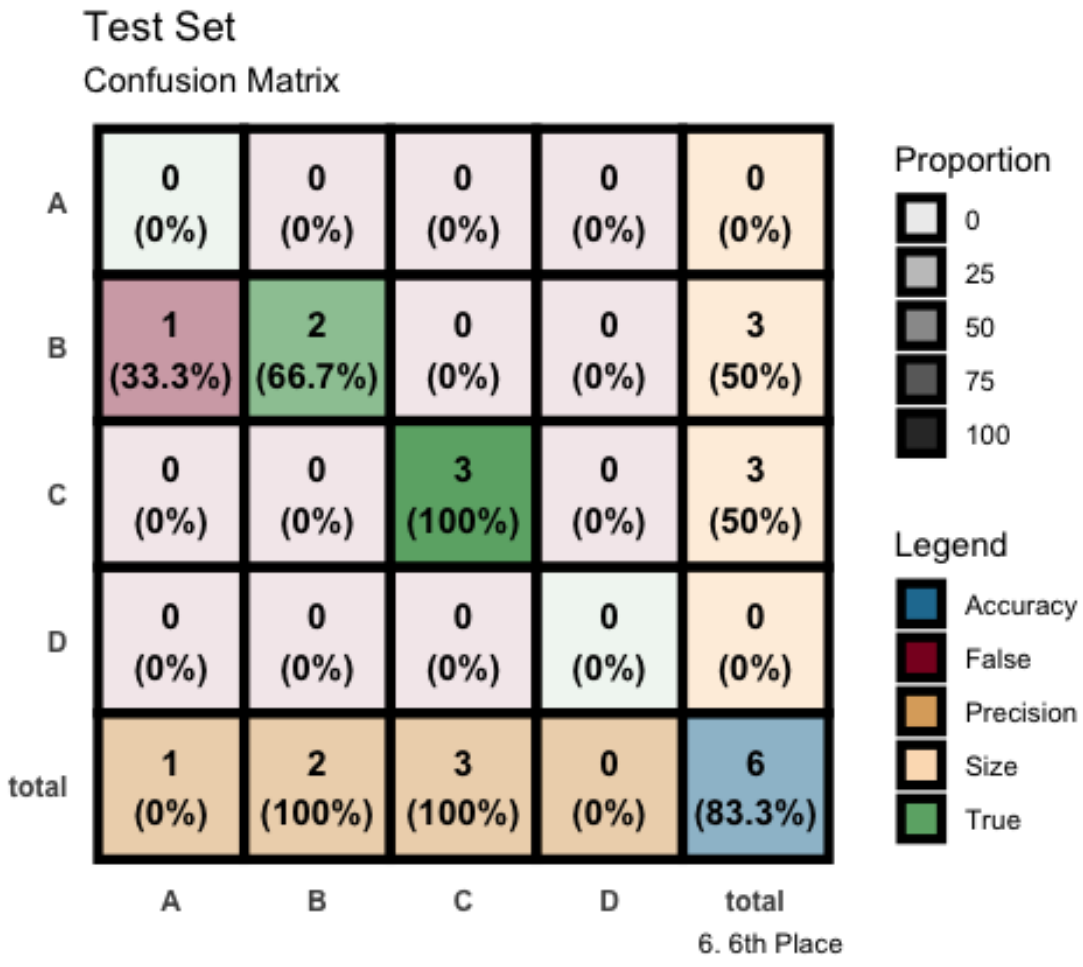
Accuracy	McFadden_R2
83.33%	0.737

Model Coefficients

	(Intercept)	fr_C_O1	fr_C_O2	fr_NH01	fr_NH02	fr_NH05	fr_NH11	fr_NH12	fr_aldehyde1
2	70.17034	-52.71775	-12.812964	-70.87779	-68.84894	-12.990123	-15.99835	-3.368135	52.88515
3	22.61667	138.16561	-7.825994	-83.29422	-38.01890	-4.075628	-115.47094	70.560126	-142.60197
4	124.86697	125.68492	49.508695	-173.75697	-124.40768	31.636503	-207.18644	-61.411756	-233.60456

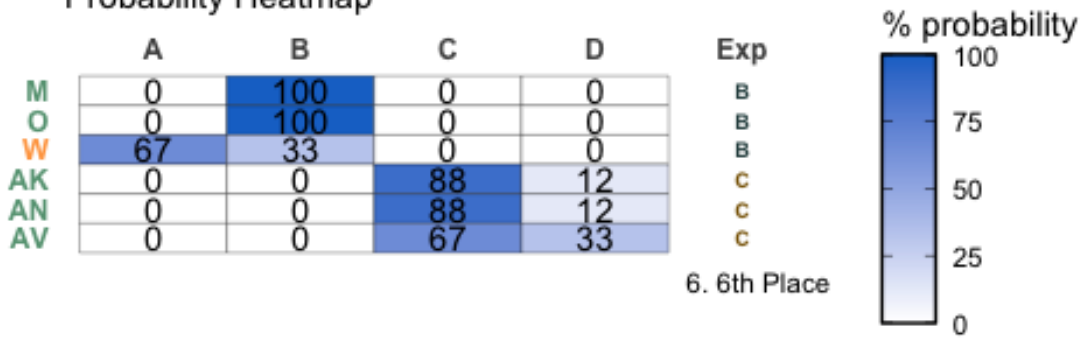

Training Set
Confusion Matrix
A
B
C
D
total
9 (90%)
1 (10%)
0 (0%)
0 (0%)
10 (20.8%)
4 (28.6%)
10 (71.4%)
0 (0%)
0 (0%)
14 (29.2%)
0 (0%)
0 (0%)
10 (100%)
0 (0%)
10 (20.8%)
0 (0%)
1 (7.1%)
2 (14.3%)
11 (78.6%)
14 (29.2%)
13 (69.2%)
12 (83.3%)
12 (83.3%)
11 (100%)
48 (83.3%)
A
B
C
D
total
6. 6th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

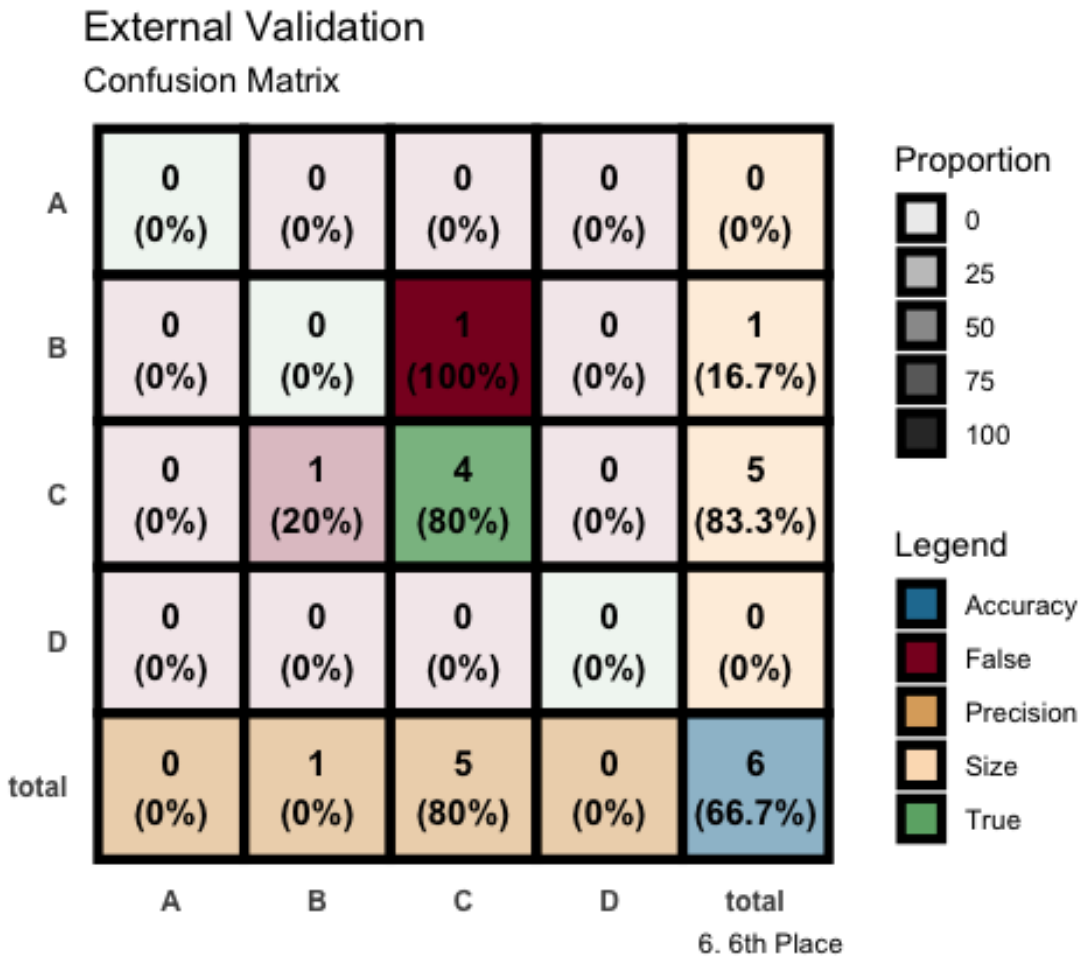

Training Set
Probability Heatmap
A
B
C
D
Exp
AF 0 0 88 12 C
AH 0 0 88 12 C
AL 0 0 88 12 C
AM 0 0 88 12 C
AO 0 0 100 0 C
AP 0 0 88 12 C
AR 0 0 67 33 C
AU 0 0 67 33 C
AW 0 0 88 12 C
AX 0 0 88 12 C
AB 18 82 0 0 B
AC 16 59 0 25 B
K 67 33 0 0 B
L 0 100 0 0 B
N 0 100 0 0 B
P 0 100 0 0 B
U 67 33 0 0 B
V 67 33 0 0 B
X 67 33 0 0 B
Z 18 82 0 0 B
AD 0 100 0 0 B
Q 0 100 0 0 B
S 0 100 0 0 B
Y 16 59 0 25 B
A 67 33 0 0 A
B 67 33 0 0 A
C 67 33 0 0 A
D 67 33 0 0 A
E 63 37 0 0 A
F 100 0 0 0 A
G 67 33 0 0 A
H 67 33 0 0 A
I 67 33 0 0 A
J 16 59 0 25 A
AZ 0 0 0 100 D
BA_rot 0 0 0 100 D
BB 0 0 0 100 D
BC 0 0 0 100 D
BD 0 0 0 100 D
BG 0 0 0 100 D
BI 0 0 0 100 D
BK 0 0 0 100 D
NM1 0 0 88 12 D
NM2 0 0 67 33 D
BE 0 0 0 100 D
BF 0 0 0 100 D
BH 0 0 0 100 D
BJ 16 59 0 25 D
% probability
100
75
50
25
0
6. 6th Place

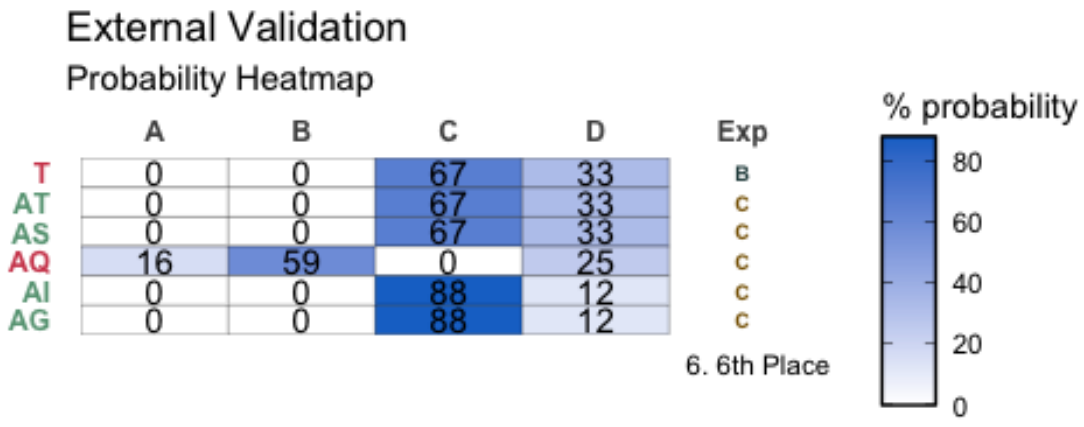

Test Set
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (33.3%)
2 (66.7%)
0 (0%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
2 (100%)
3 (100%)
0 (0%)
6 (83.3%)
A
B
C
D
total
6. 6th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Test Set

Probability Heatmap




External Validation
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (100%)
0 (0%)
1 (16.7%)
0 (0%)
1 (20%)
4 (80%)
0 (0%)
5 (83.3%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
5 (80%)
0 (0%)
6 (66.7%)
A
B
C
D
total
6. 6th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True


External Validation
Probability Heatmap
A
B
C
D
Exp
T
AT
AS
AQ
AI
AG
0 0 67 33 B
0 0 67 33 C
0 0 67 33 C
16 59 0 25 C
0 0 88 12 C
0 0 88 12 C
6. 6th Place
% probability
80
60
40
20
0

7th Place

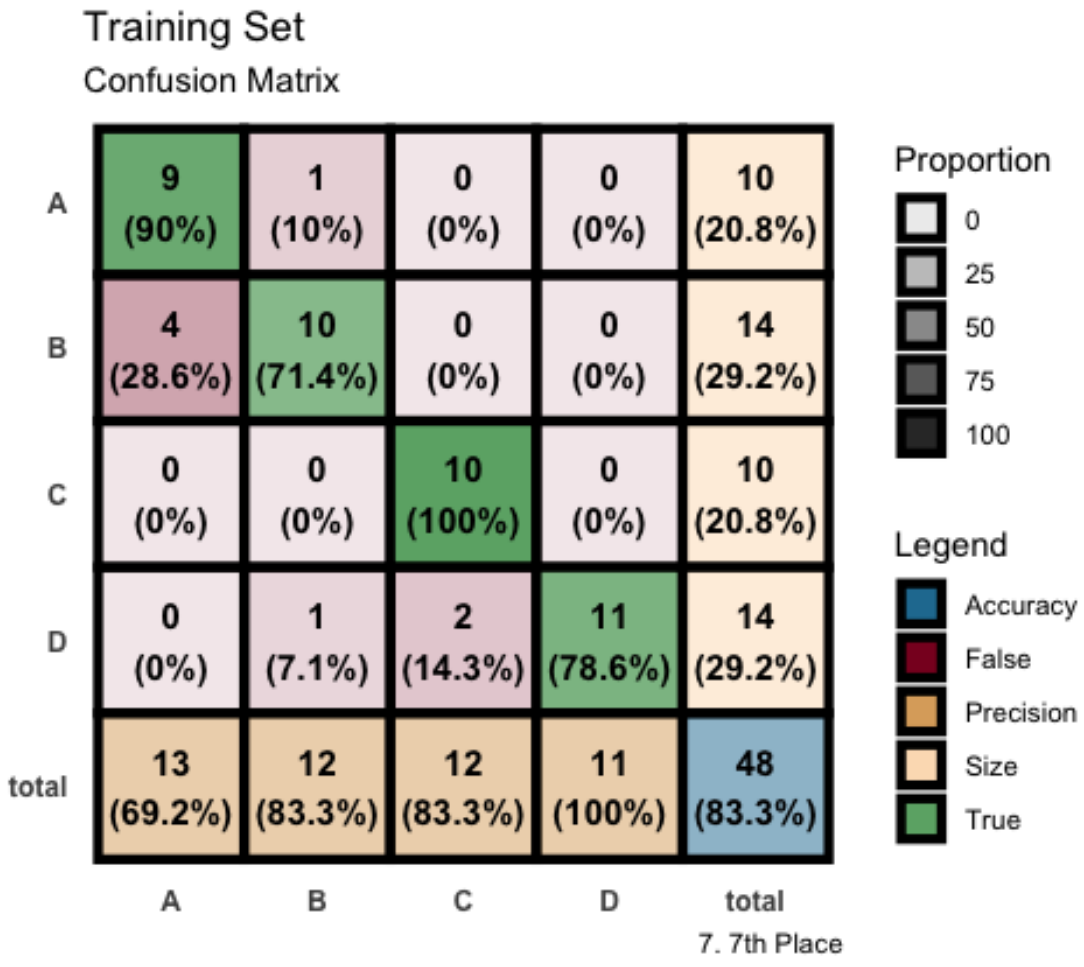
Table:

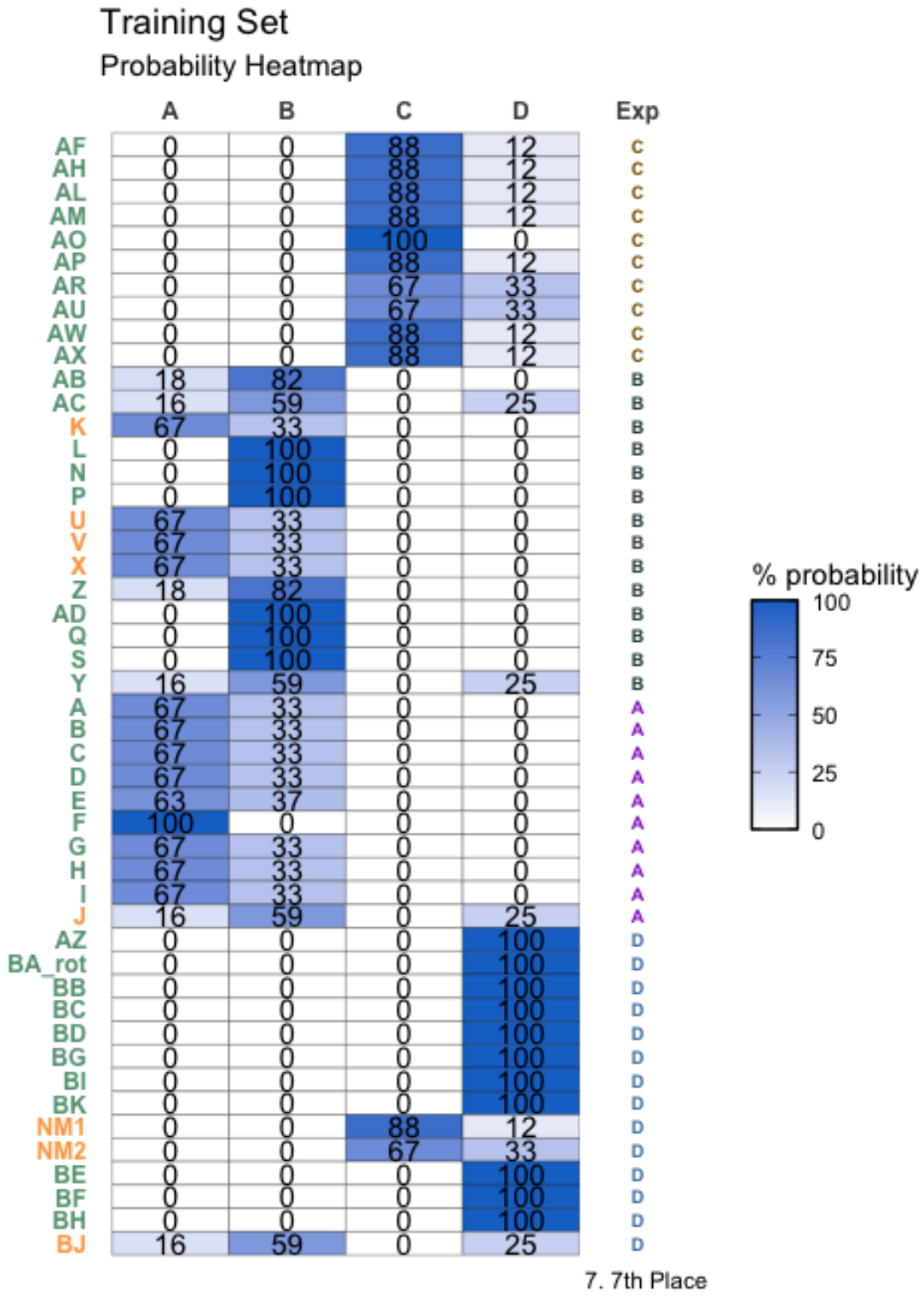
Full Model Stats - Overall Accuracy and Pseudo-R2

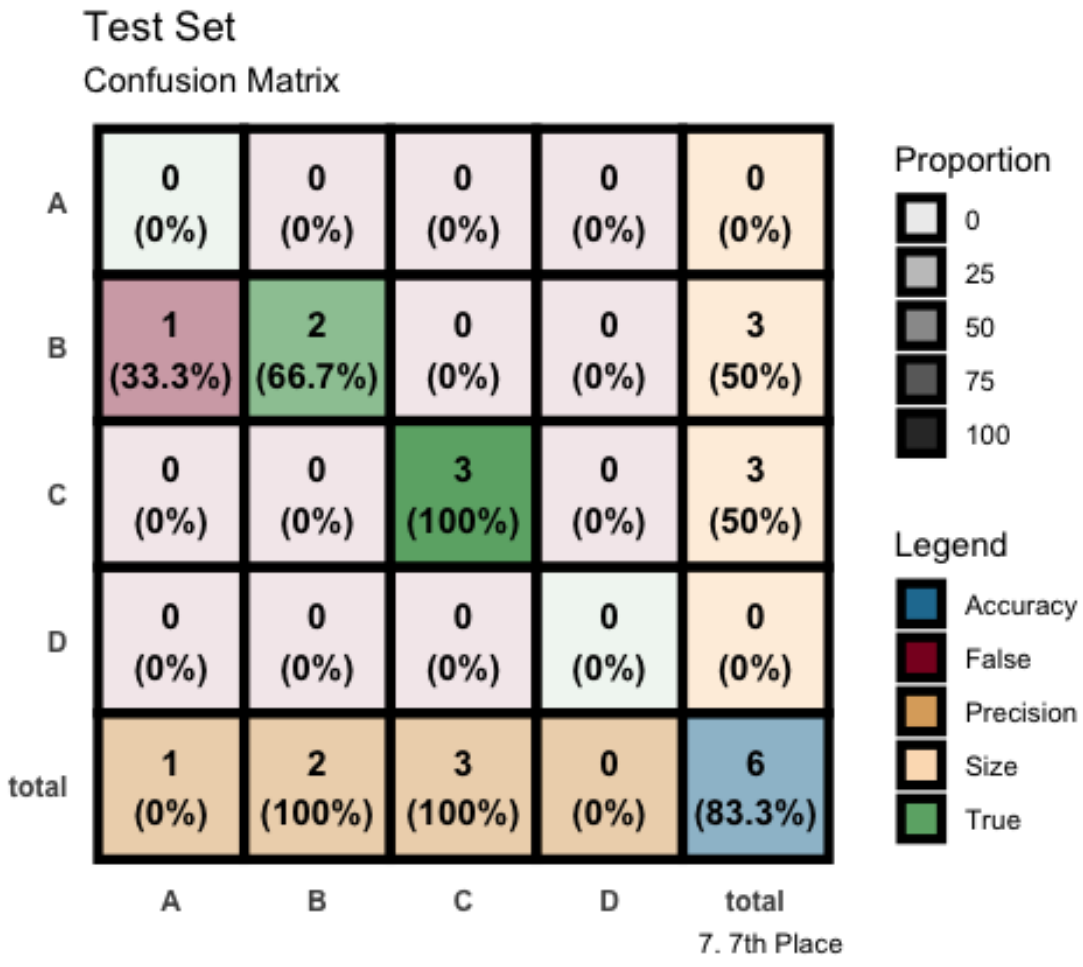
Accuracy	McFadden_R2
83.33%	0.737

Model Coefficients

	(Intercept)	fr_C_O_noCOO1	fr_C_O_noCOO2	fr_NH01	fr_NH02	fr_NH05	fr_NH11	fr_NH12	fr_aldehyde1
2	54.736286	-44.66841	-7.795743	-55.44372	-53.41487	-9.879302	-13.40997	-2.70421	44.83582
3	9.113925	104.58178	-6.811975	-59.28324	-24.74341	-3.523018	-83.05231	65.30208	-117.93056
4	105.673656	104.12244	38.198808	-156.07682	-105.21437	24.612613	-181.09863	-57.61870	-178.98233

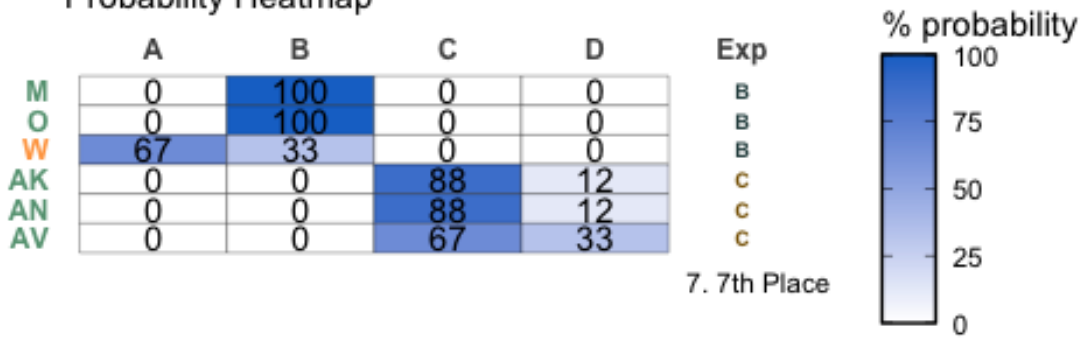

Training Set
Confusion Matrix
A
B
C
D
total
9 (90%)
1 (10%)
0 (0%)
0 (0%)
10 (20.8%)
4 (28.6%)
10 (71.4%)
0 (0%)
0 (0%)
14 (29.2%)
0 (0%)
0 (0%)
10 (100%)
0 (0%)
10 (20.8%)
0 (0%)
1 (7.1%)
2 (14.3%)
11 (78.6%)
14 (29.2%)
13 (69.2%)
12 (83.3%)
12 (83.3%)
11 (100%)
48 (83.3%)
A
B
C
D
total
7. 7th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

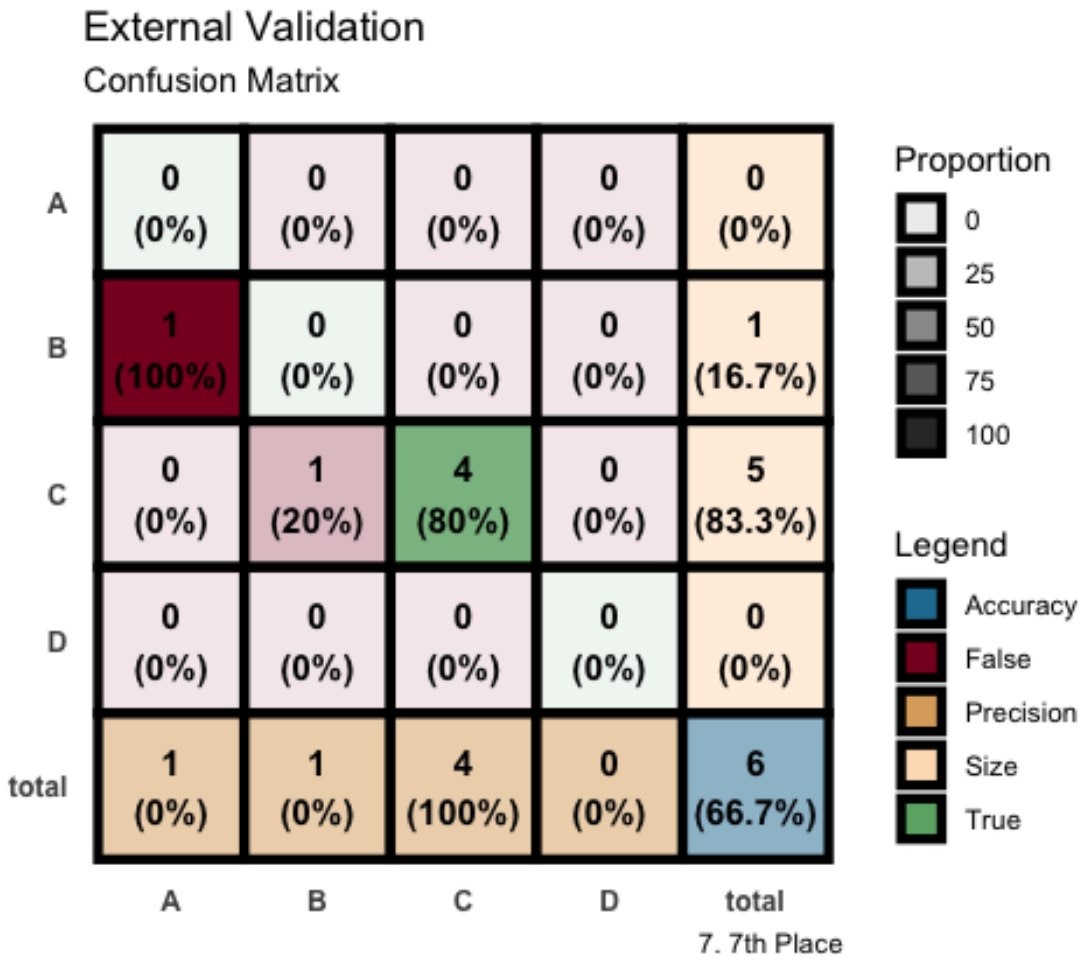

Training Set
Probability Heatmap
A
B
C
D
Exp
AF 0 0 88 12 C
AH 0 0 88 12 C
AL 0 0 88 12 C
AM 0 0 88 12 C
AO 0 0 100 0 C
AP 0 0 88 12 C
AR 0 0 67 33 C
AU 0 0 67 33 C
AW 0 0 88 12 C
AX 0 0 88 12 C
AB 18 82 0 0 B
AC 16 59 0 25 B
K 67 33 0 0 B
L 0 100 0 0 B
N 0 100 0 0 B
P 0 100 0 0 B
U 67 33 0 0 B
V 67 33 0 0 B
X 67 33 0 0 B
Z 18 82 0 0 B
AD 0 100 0 0 B
Q 0 100 0 0 B
S 0 100 0 0 B
Y 16 59 0 25 B
A 67 33 0 0 A
B 67 33 0 0 A
C 67 33 0 0 A
D 67 33 0 0 A
E 63 37 0 0 A
F 100 0 0 0 A
G 67 33 0 0 A
H 67 33 0 0 A
I 67 33 0 0 A
J 16 59 0 25 A
AZ 0 0 0 100 D
BA_rot 0 0 0 100 D
BB 0 0 0 100 D
BC 0 0 0 100 D
BD 0 0 0 100 D
BG 0 0 0 100 D
BI 0 0 0 100 D
BK 0 0 0 100 D
NM1 0 0 88 12 D
NM2 0 0 67 33 D
BE 0 0 0 100 D
BF 0 0 0 100 D
BH 0 0 0 100 D
BJ 16 59 0 25 D
% probability
100
75
50
25
0
7. 7th Place

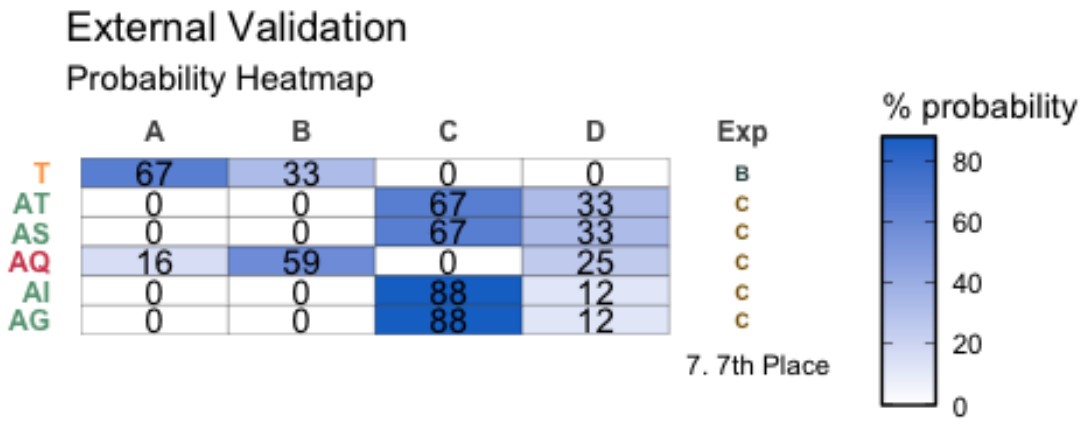

Test Set
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (33.3%)
2 (66.7%)
0 (0%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
2 (100%)
3 (100%)
0 (0%)
6 (83.3%)
A
B
C
D
total
7. 7th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Test Set

Probability Heatmap




External Validation
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (100%)
0 (0%)
0 (0%)
0 (0%)
1 (16.7%)
0 (0%)
1 (20%)
4 (80%)
0 (0%)
5 (83.3%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
1 (0%)
4 (100%)
0 (0%)
6 (66.7%)
A
B
C
D
total
7. 7th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True


External Validation
Probability Heatmap
A
B
C
D
Exp
T
AT
AS
AQ
AI
AG
67
33
0
0
0
0
67
33
0
0
67
33
16
59
0
25
0
0
88
12
0
0
88
12
B
C
C
C
C
C
7. 7th Place
% probability
80
60
40
20
0

8th Place

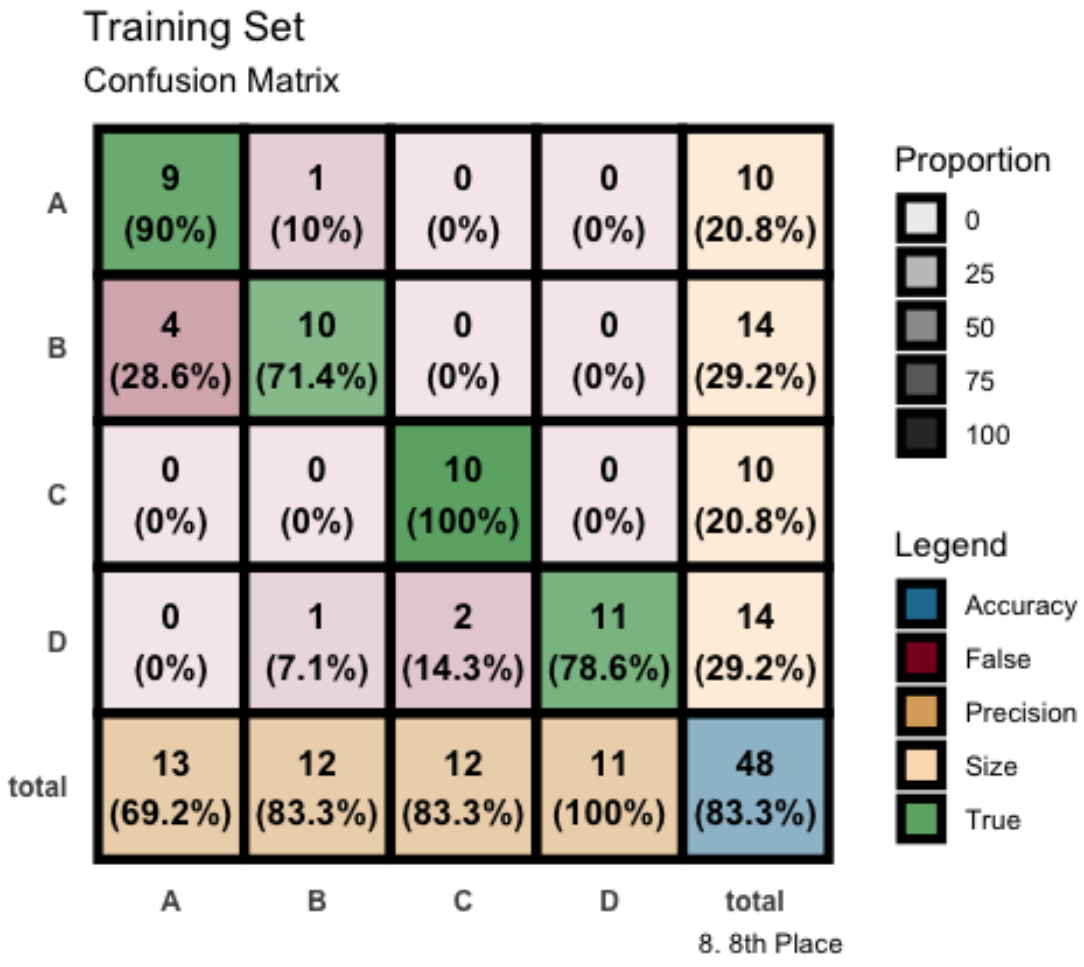
Table:

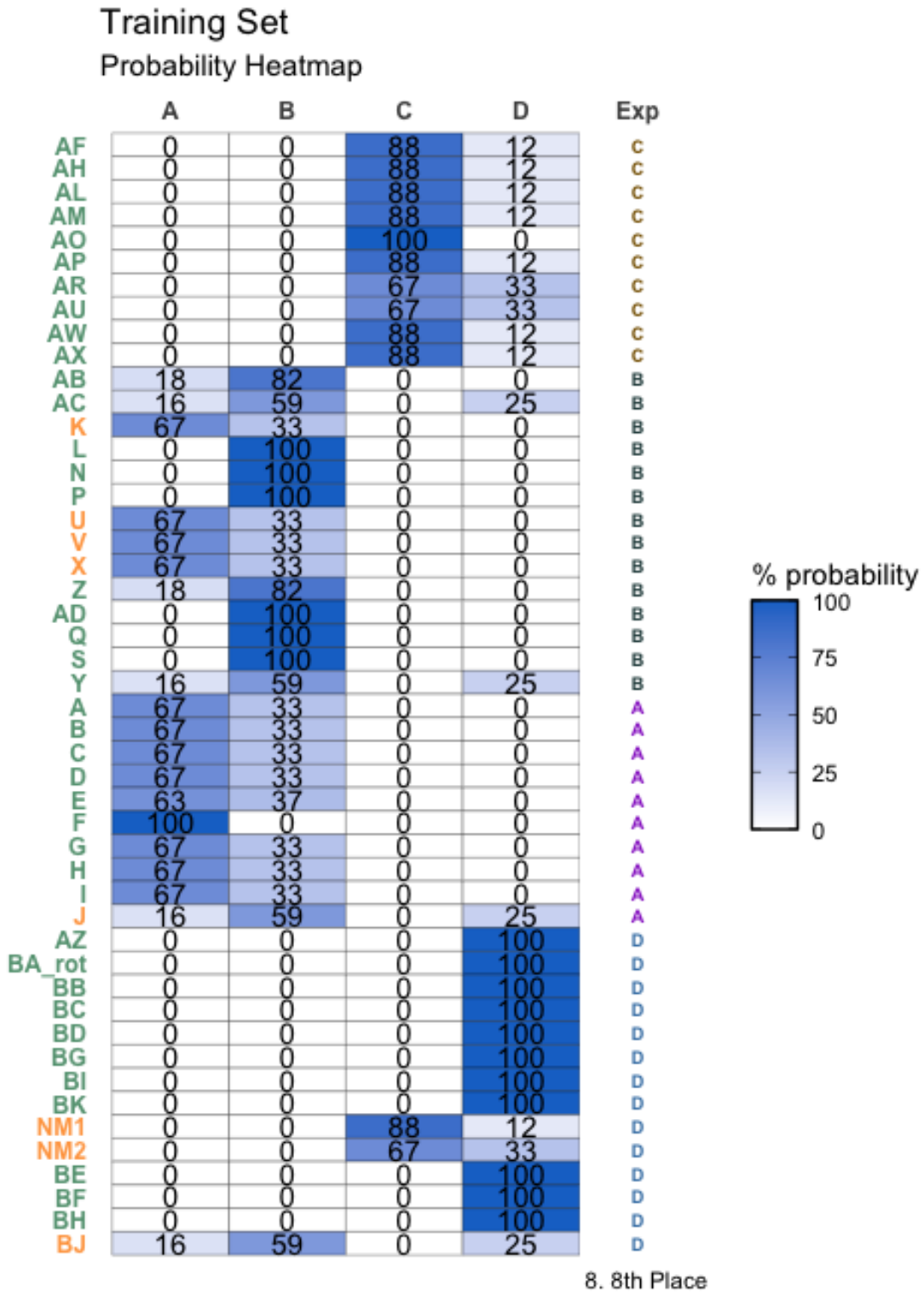
Full Model Stats - Overall Accuracy and Pseudo-R2

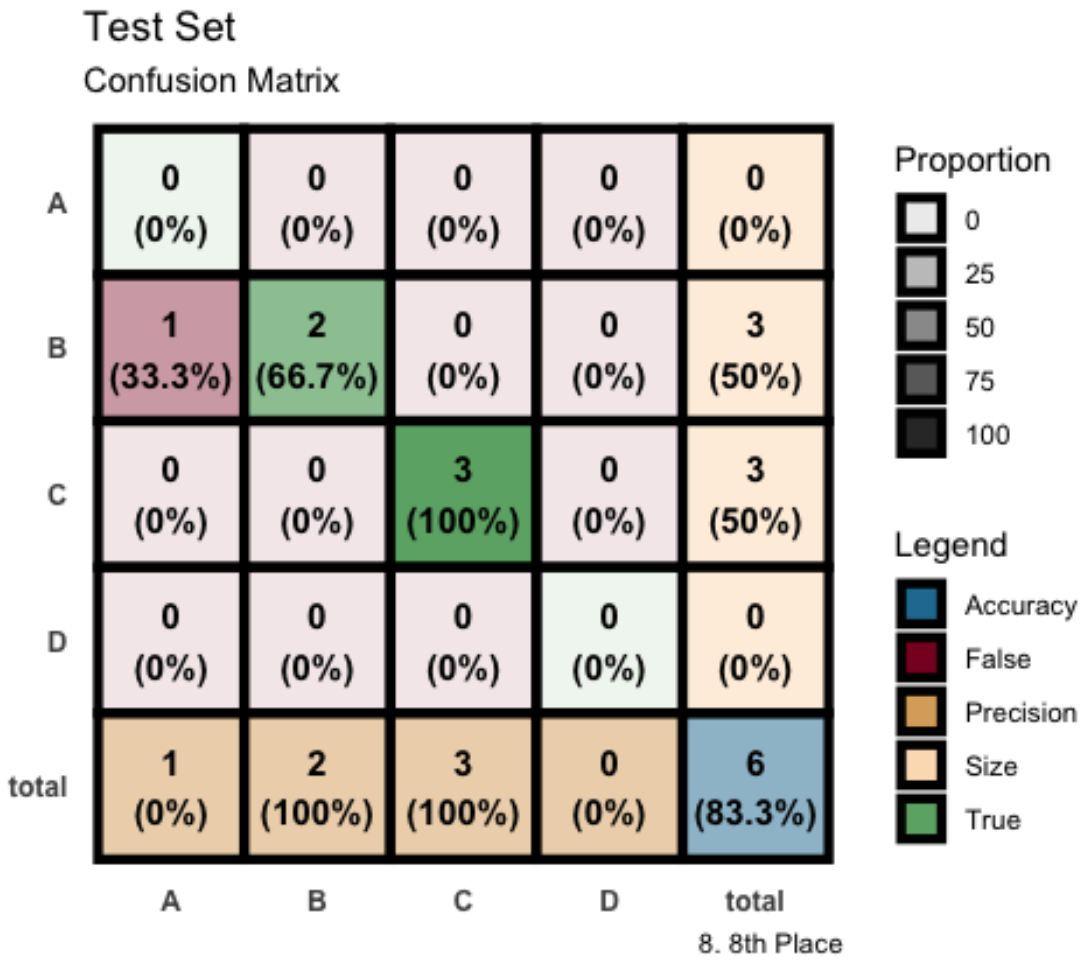
Accuracy	McFadden_R2
83.33%	0.737

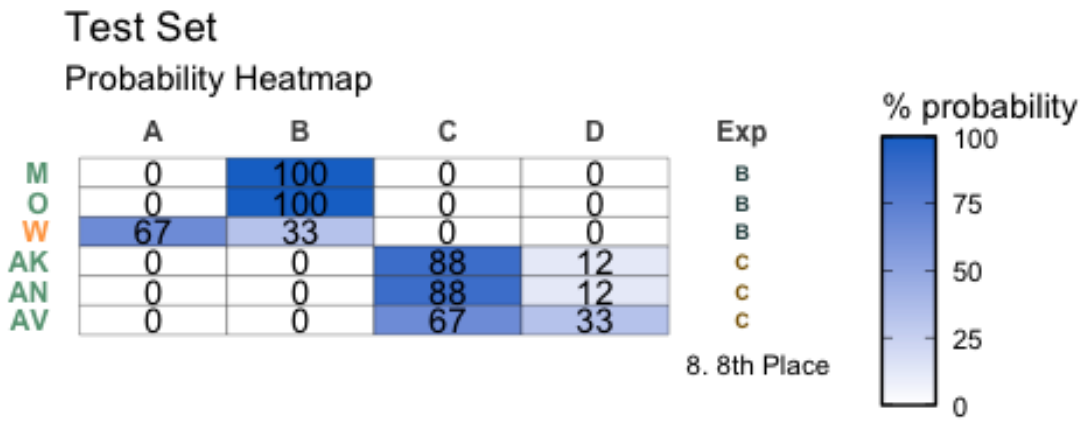
Model Coefficients

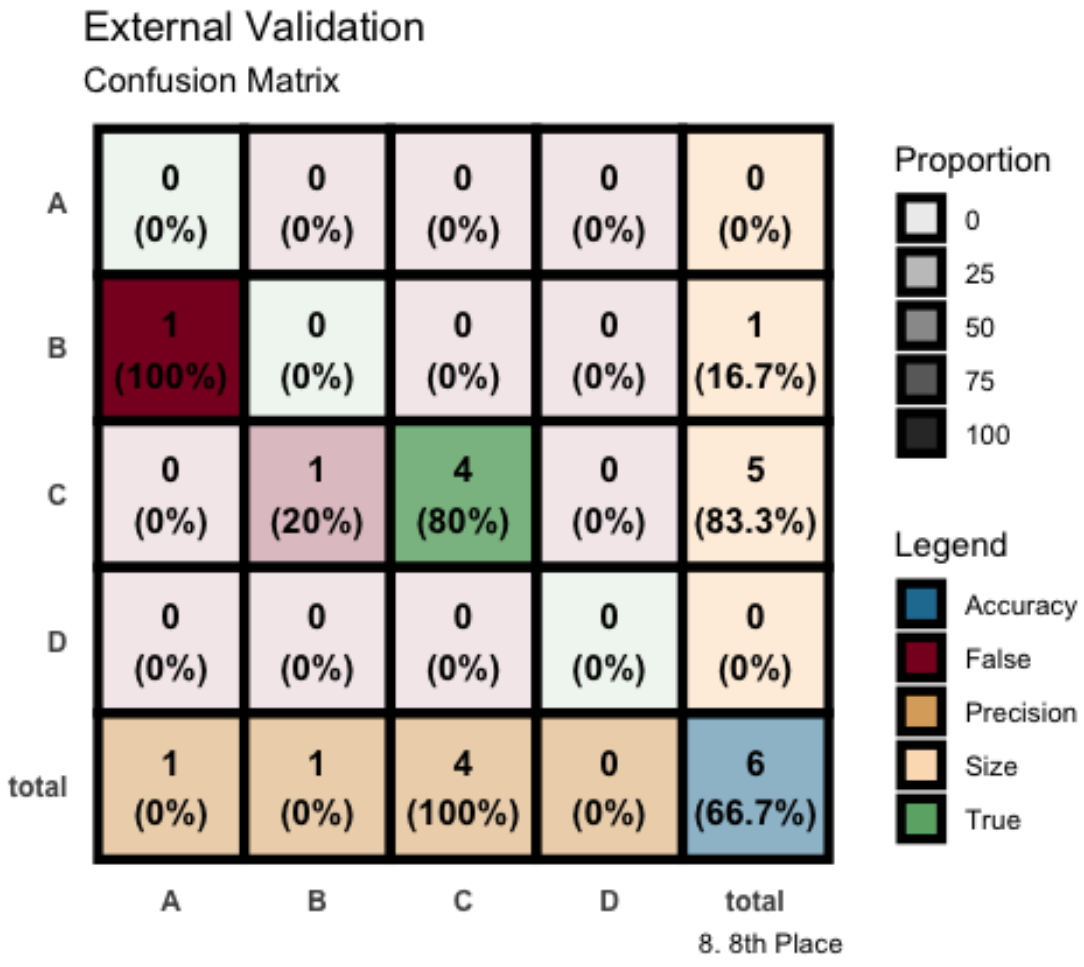
	(Intercept)	fr_NH01	fr_NH02	fr_NH05	fr_NH11	fr_NH12	fr_aldehyde1	fr_amide1	fr_amide2
2	60.70480	-61.41225	-59.38359	-6.888058	3.123181	-9.996372	0.1676192	-41.44892	-9.996372
3	27.87299	-84.46899	-43.58631	-2.482707	-104.292953	57.808035	-63.8560158	119.18717	57.808035
4	90.29337	-128.64724	-89.83429	17.764335	-149.723994	-32.920594	-123.5222002	100.25195	-32.920594

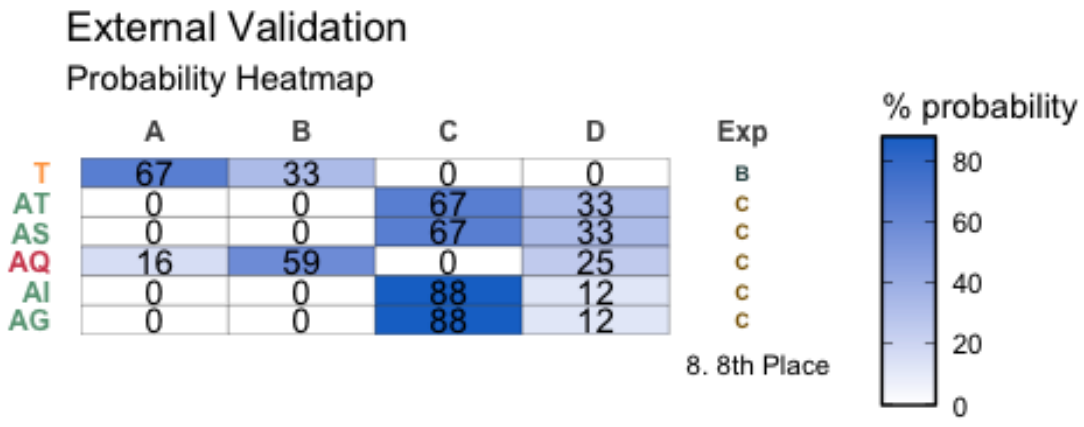

Training Set
Confusion Matrix
A
B
C
D
total
9 (90%)
1 (10%)
0 (0%)
0 (0%)
10 (20.8%)
4 (28.6%)
10 (71.4%)
0 (0%)
0 (0%)
14 (29.2%)
0 (0%)
0 (0%)
10 (100%)
0 (0%)
10 (20.8%)
0 (0%)
1 (7.1%)
2 (14.3%)
11 (78.6%)
14 (29.2%)
13 (69.2%)
12 (83.3%)
12 (83.3%)
11 (100%)
48 (83.3%)
A
B
C
D
total
8. 8th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True


Training Set
Probability Heatmap
A
B
C
D
Exp
AF 0 0 88 12 C
AH 0 0 88 12 C
AL 0 0 88 12 C
AM 0 0 88 12 C
AO 0 0 100 0 C
AP 0 0 88 12 C
AR 0 0 67 33 C
AU 0 0 67 33 C
AW 0 0 88 12 C
AX 0 0 88 12 C
AB 18 82 0 0 B
AC 16 59 0 25 B
K 67 33 0 0 B
L 0 100 0 0 B
N 0 100 0 0 B
P 0 100 0 0 B
U 67 33 0 0 B
V 67 33 0 0 B
X 67 33 0 0 B
Z 18 82 0 0 B
AD 0 100 0 0 B
Q 0 100 0 0 B
S 0 100 0 0 B
Y 16 59 0 25 B
A 67 33 0 0 A
B 67 33 0 0 A
C 67 33 0 0 A
D 67 33 0 0 A
E 63 37 0 0 A
F 100 0 0 0 A
G 67 33 0 0 A
H 67 33 0 0 A
I 67 33 0 0 A
J 16 59 0 25 A
AZ 0 0 0 100 D
BA_rot 0 0 0 100 D
BB 0 0 0 100 D
BC 0 0 0 100 D
BD 0 0 0 100 D
BG 0 0 0 100 D
BI 0 0 0 100 D
BK 0 0 0 100 D
NM1 0 0 88 12 D
NM2 0 0 67 33 D
BE 0 0 0 100 D
BF 0 0 0 100 D
BH 0 0 0 100 D
BJ 16 59 0 25 D
% probability
100
75
50
25
0
8. 8th Place


Test Set
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (33.3%)
2 (66.7%)
0 (0%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
2 (100%)
3 (100%)
0 (0%)
6 (83.3%)
A
B
C
D
total
8. 8th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True


Test Set
Probability Heatmap
A
B
C
D
Exp
M
O
W
AK
AN
AV
0
100
0
0
B
0
100
0
0
B
67
33
0
0
B
0
0
88
12
C
0
0
88
12
C
0
0
67
33
C
8. 8th Place
% probability
100
75
50
25
0


External Validation
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (100%)
0 (0%)
0 (0%)
0 (0%)
1 (16.7%)
0 (0%)
1 (20%)
4 (80%)
0 (0%)
5 (83.3%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
1 (0%)
4 (100%)
0 (0%)
6 (66.7%)
A
B
C
D
total
8. 8th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True


External Validation
Probability Heatmap
A
B
C
D
Exp
T
AT
AS
AQ
AI
AG
67
33
0
0
0
0
67
33
0
0
67
33
16
59
0
25
0
0
88
12
0
0
88
12
B
C
C
C
C
C
8. 8th Place
% probability
80
60
40
20
0

9th Place

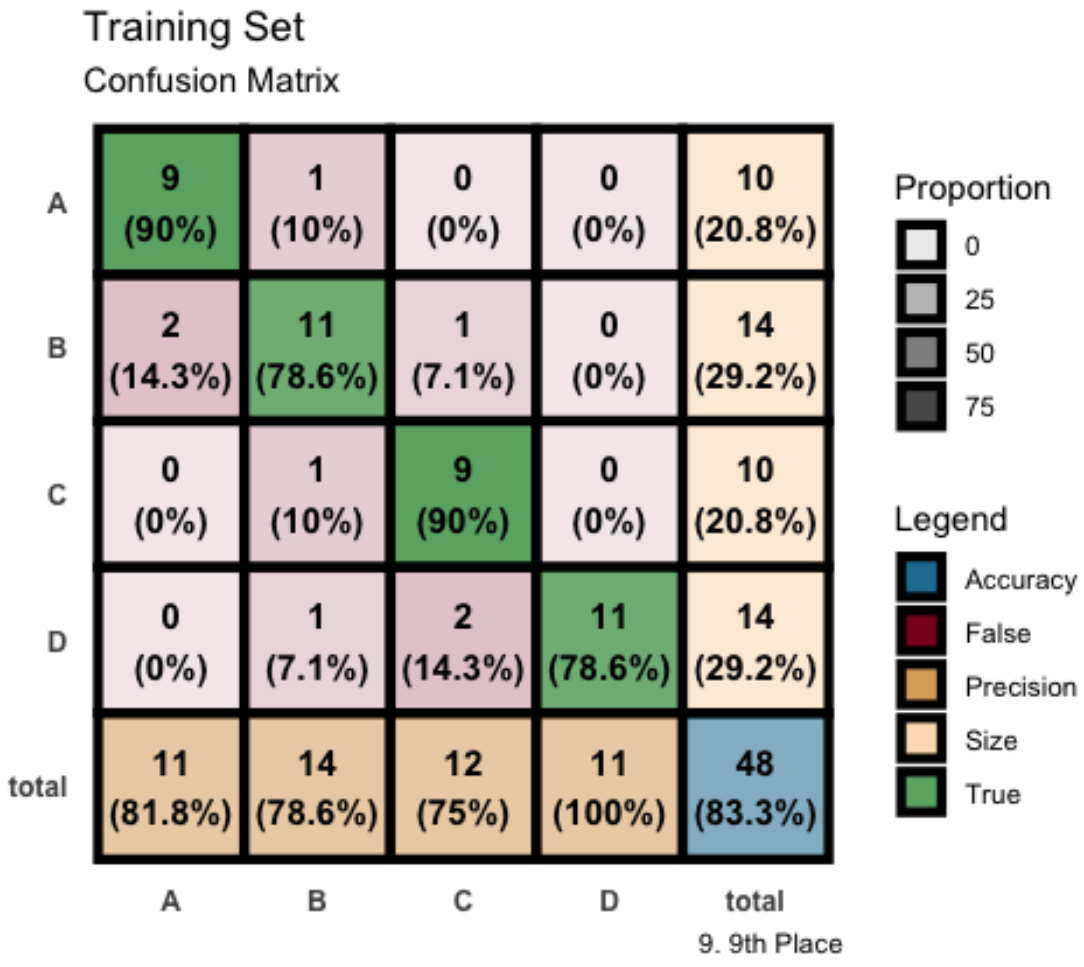
Table:

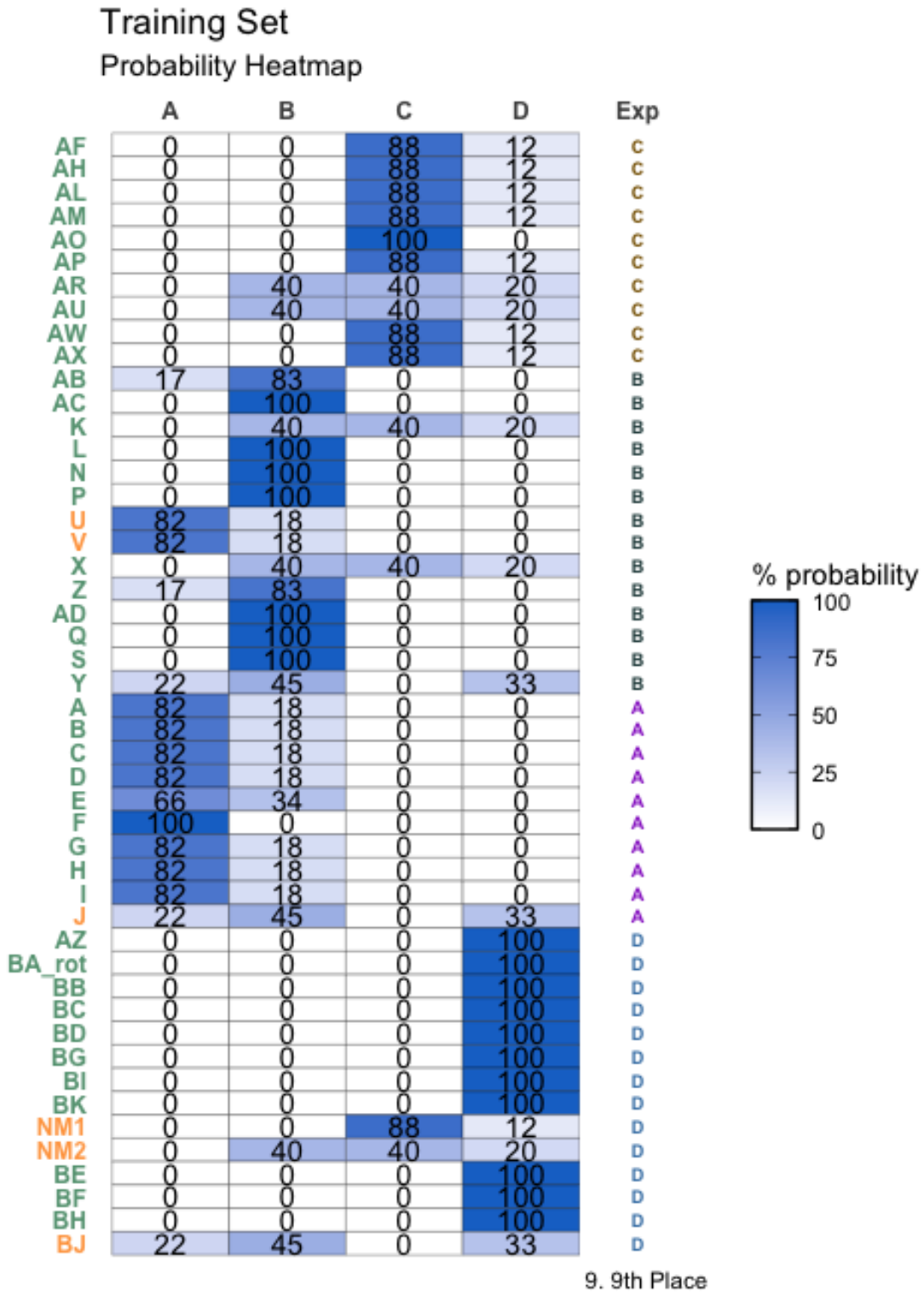
Full Model Stats - Overall Accuracy and Pseudo-R2

Accuracy	McFadden_R2
83.33%	0.737

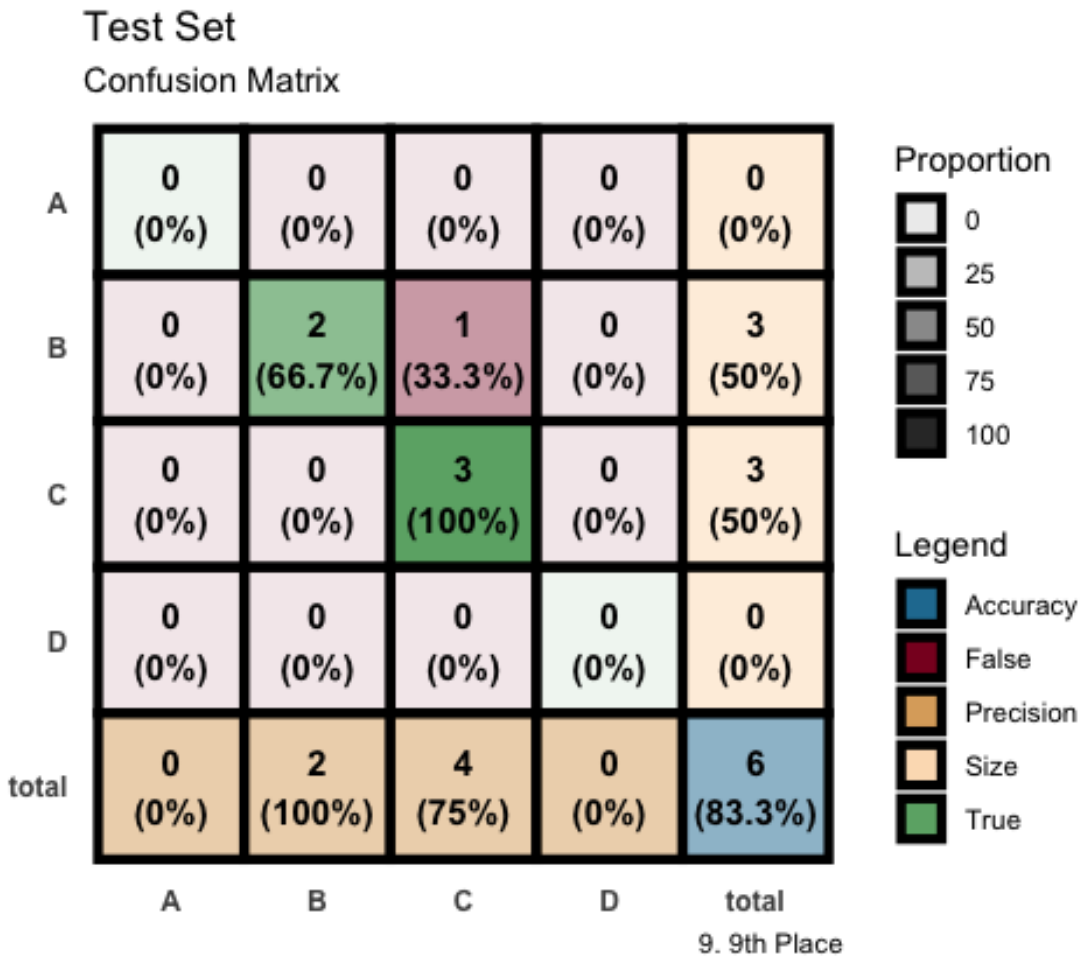
Model Coefficients

	(Intercept)	fr_NH01	fr_NH02	fr_NH05	fr_NH11	fr_NH12	fr_aldehyde1	fr_pyridine1	fr_pyridine2
2	38.89929	5.181797	-38.18001	-4.448289	-23.86882	-7.412637	0.8489931	-45.57125	39.156240
3	13.24098	30.840104	-44.97720	-3.342463	34.62293	45.949696	-55.66462	-98.22449	-2.993153
4	72.32253	-28.934631	-71.89964	11.003202	-26.40458	-33.256233	-102.6309141	-84.26565	-17.478519


Training Set
Confusion Matrix
A
B
C
D
total
9 (90%)
1 (10%)
0 (0%)
0 (0%)
10 (20.8%)
2 (14.3%)
11 (78.6%)
1 (7.1%)
0 (0%)
14 (29.2%)
0 (0%)
1 (10%)
9 (90%)
0 (0%)
10 (20.8%)
0 (0%)
1 (7.1%)
2 (14.3%)
11 (78.6%)
14 (29.2%)
11 (81.8%)
14 (78.6%)
12 (75%)
11 (100%)
48 (83.3%)
A
B
C
D
total
9. 9th Place
Proportion
0
25
50
75
Legend
Accuracy
False
Precision
Size
True

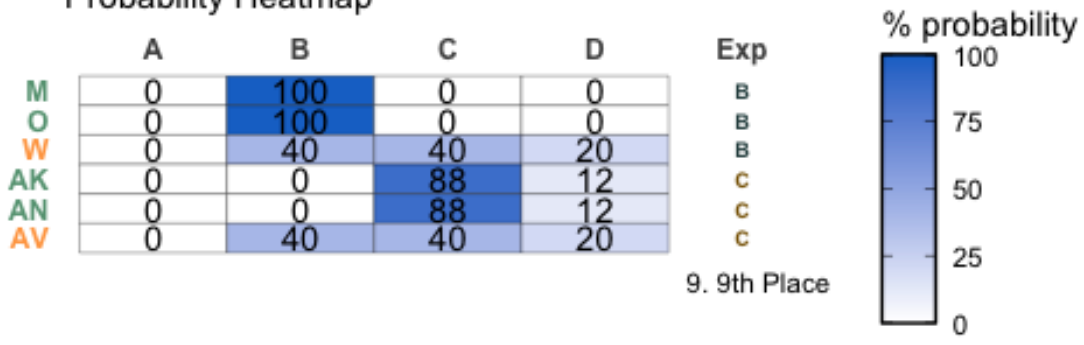

Training Set
Probability Heatmap
A
B
C
D
Exp
AF 0 0 88 12 C
AH 0 0 88 12 C
AL 0 0 88 12 C
AM 0 0 88 12 C
AO 0 0 100 0 C
AP 0 0 88 12 C
AR 0 40 40 20 C
AU 0 40 40 20 C
AW 0 0 88 12 C
AX 0 0 88 12 C
AB 17 83 0 0 B
AC 0 100 0 0 B
K 0 40 40 20 B
L 0 100 0 0 B
N 0 100 0 0 B
P 0 100 0 0 B
U 82 18 0 0 B
V 82 18 0 0 B
X 0 40 40 20 B
Z 17 83 0 0 B
AD 0 100 0 0 B
Q 0 100 0 0 B
S 0 100 0 0 B
Y 22 45 0 33 B
A 82 18 0 0 A
B 82 18 0 0 A
C 82 18 0 0 A
D 82 18 0 0 A
E 66 34 0 0 A
F 100 0 0 0 A
G 82 18 0 0 A
H 82 18 0 0 A
I 82 18 0 0 A
J 22 45 0 33 A
AZ 0 0 0 100 D
BA_rot 0 0 0 100 D
BB 0 0 0 100 D
BC 0 0 0 100 D
BD 0 0 0 100 D
BG 0 0 0 100 D
BI 0 0 0 100 D
BK 0 0 0 100 D
NM1 0 0 88 12 D
NM2 0 40 40 20 D
BE 0 0 0 100 D
BF 0 0 0 100 D
BH 0 0 0 100 D
BJ 22 45 0 33 D
% probability
100
75
50
25
0

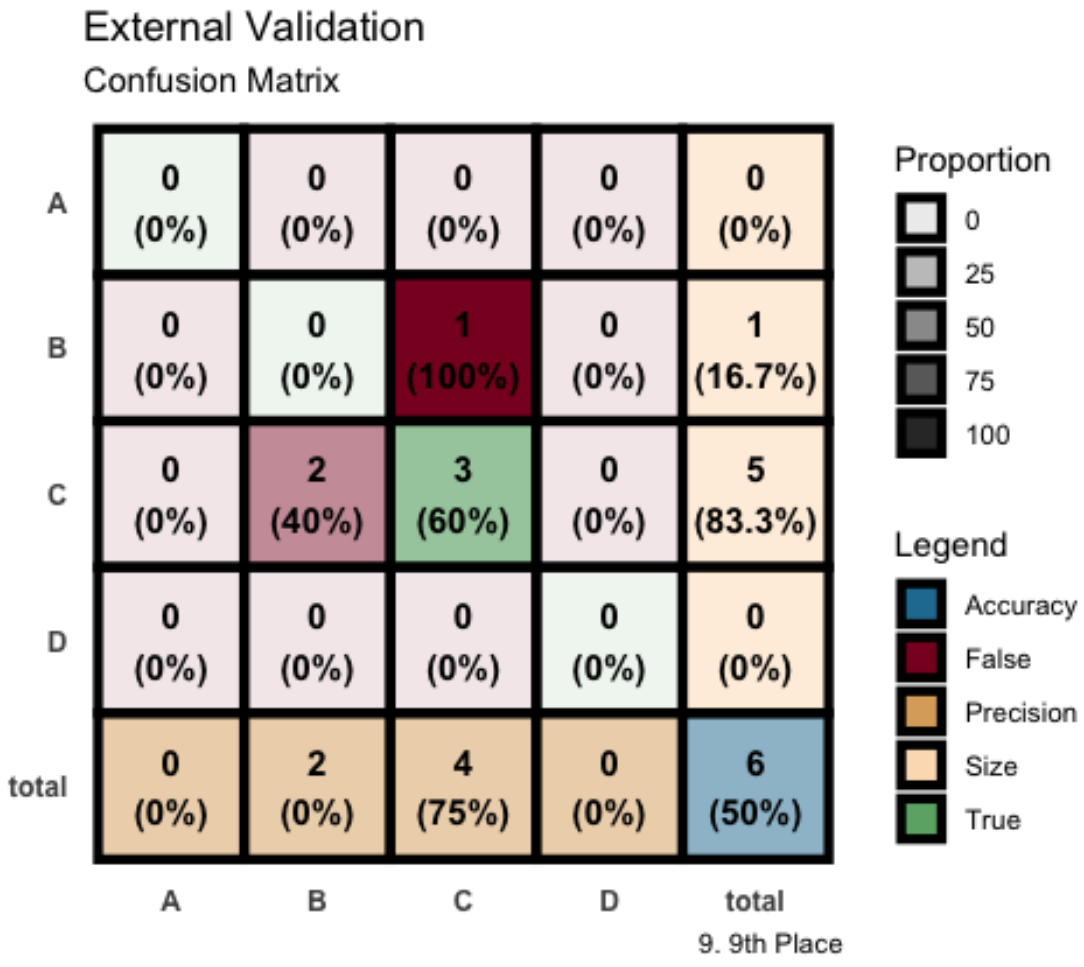
9. 9th Place


Test Set
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
2 (66.7%)
1 (33.3%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
2 (100%)
4 (75%)
0 (0%)
6 (83.3%)
A
B
C
D
total
9. 9th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

Test Set

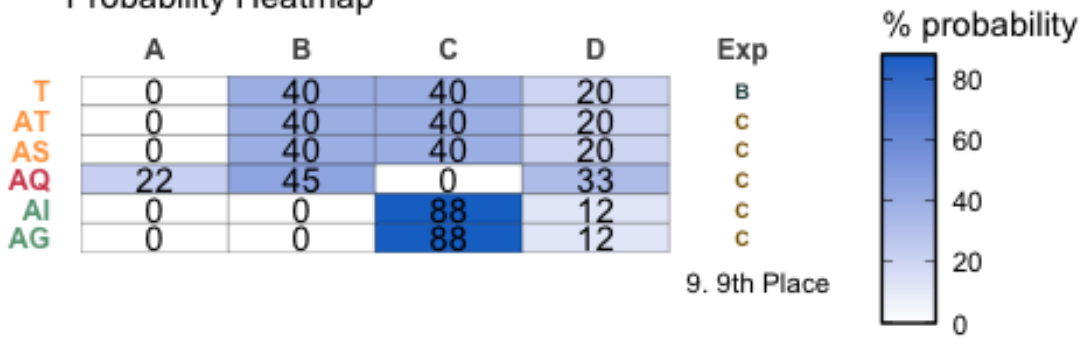
Probability Heatmap




External Validation
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (100%)
0 (0%)
1 (16.7%)
0 (0%)
2 (40%)
3 (60%)
0 (0%)
5 (83.3%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
2 (0%)
4 (75%)
0 (0%)
6 (50%)
A
B
C
D
total
9. 9th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

External Validation

Probability Heatmap



10th Place

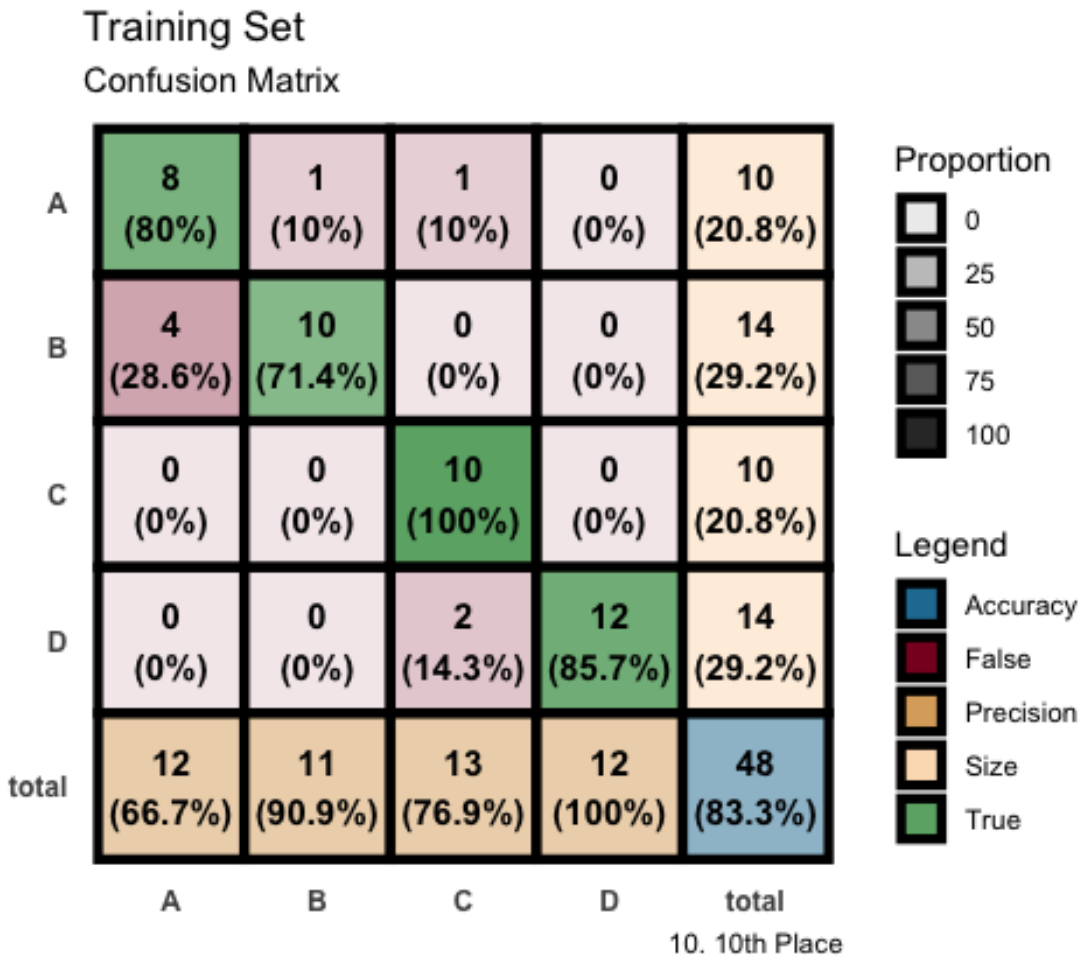
Table:

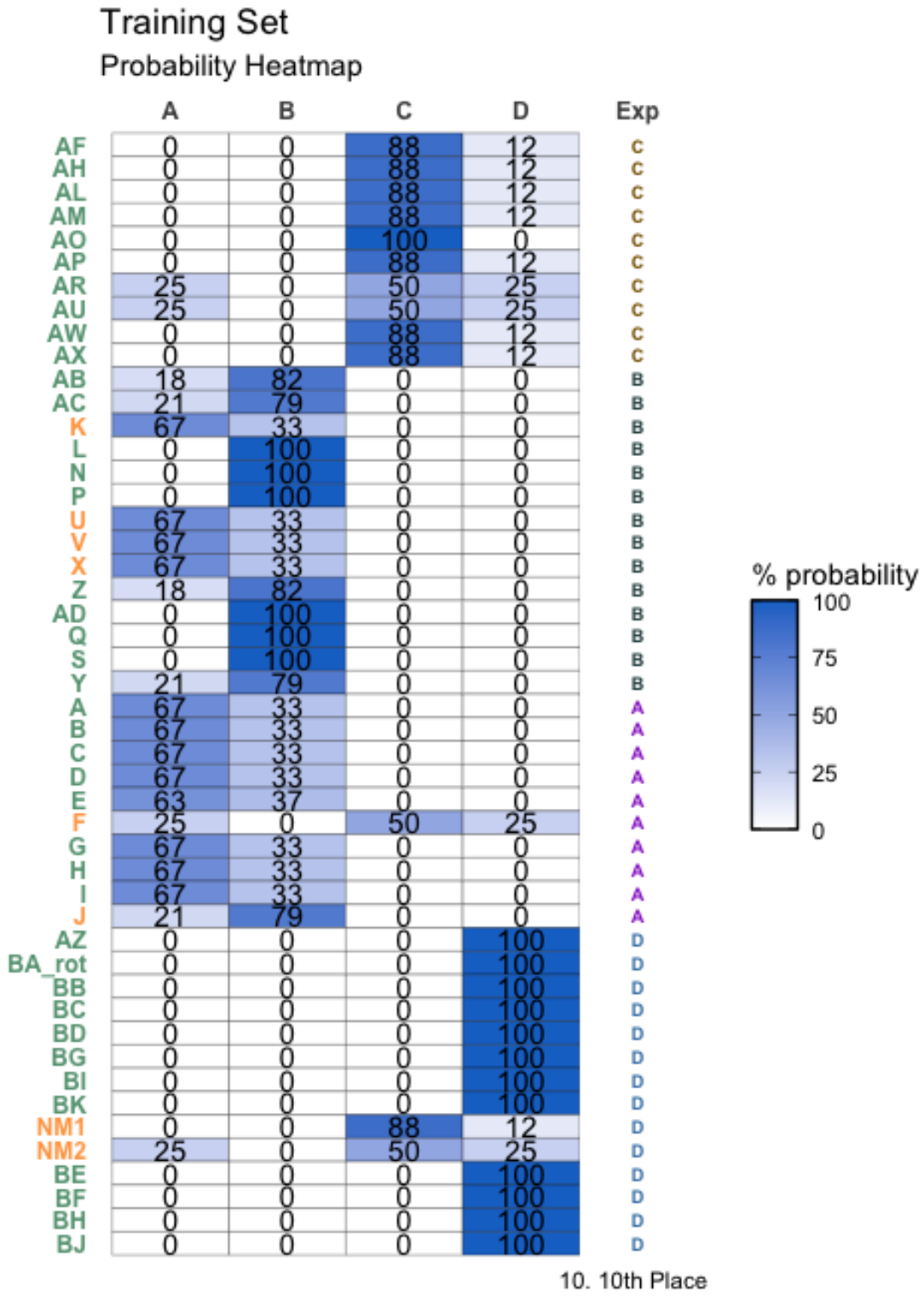
Full Model Stats - Overall Accuracy and Pseudo-R2

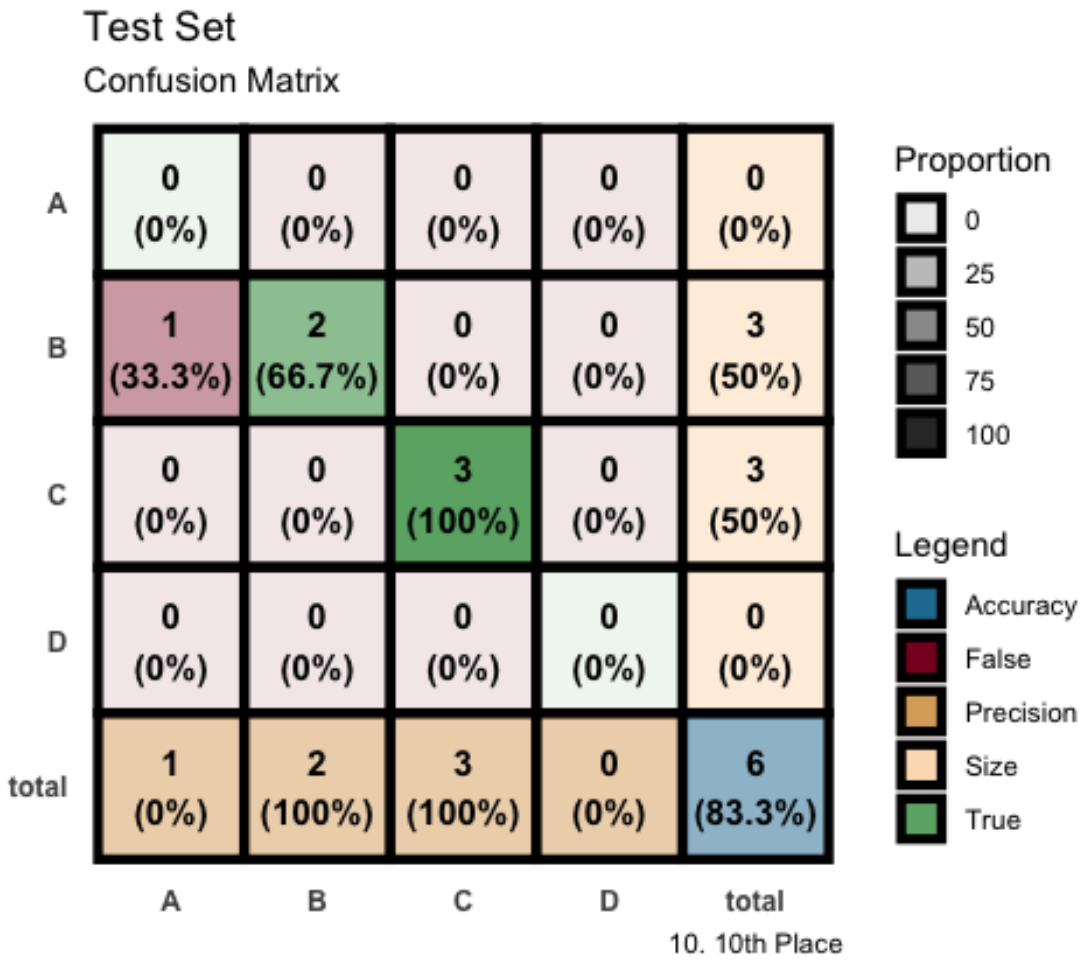
Accuracy	McFadden_R2
83.33%	0.737

Model Coefficients

	(Intercept)	fr_NH01	fr_NH02	fr_NH05	fr_NH21	fr_aldehyde1	fr_amide1	fr_amide2
2	42.460572	-43.16802	-41.13927	-6.911364	-23.42086	0.167515	-21.43447	-10.56109
3	9.360216	-93.61364	-25.16568	-3.070832	-15.48587	-103.845171	84.94657	65.75334
4	63.644940	-92.36085	-80.48895	19.213711	63.31724	-106.463677	28.71593	-41.81901

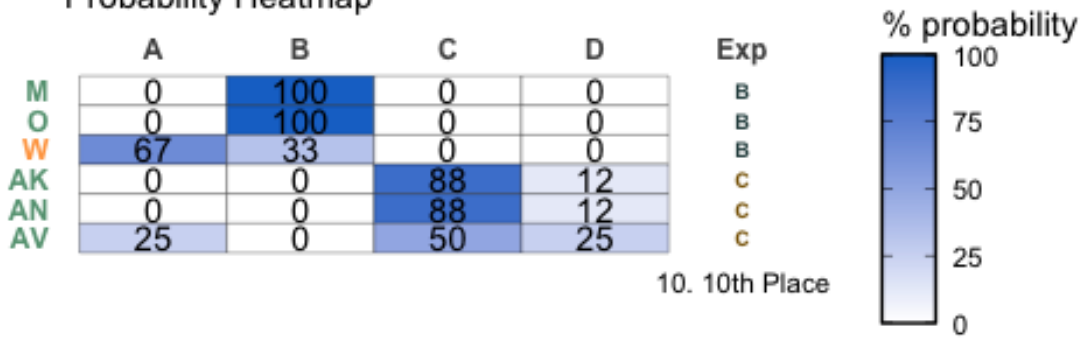

Training Set
Confusion Matrix
A
B
C
D
total
8 (80%)
1 (10%)
1 (10%)
0 (0%)
10 (20.8%)
4 (28.6%)
10 (71.4%)
0 (0%)
0 (0%)
14 (29.2%)
0 (0%)
0 (0%)
10 (100%)
0 (0%)
10 (20.8%)
0 (0%)
0 (0%)
2 (14.3%)
12 (85.7%)
14 (29.2%)
12 (66.7%)
11 (90.9%)
13 (76.9%)
12 (100%)
48 (83.3%)
A
B
C
D
total
10. 10th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

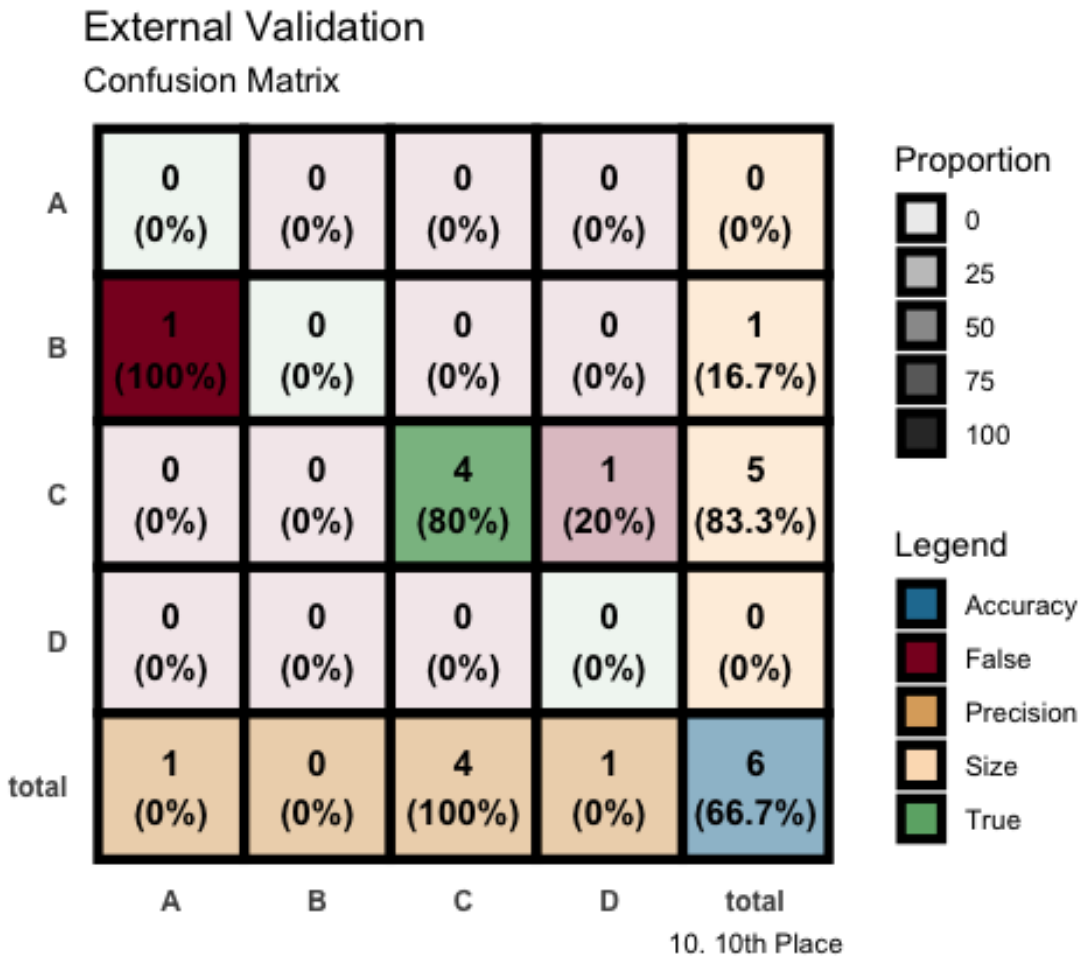

Training Set
Probability Heatmap
A
B
C
D
Exp
AF 0 0 88 12 C
AH 0 0 88 12 C
AL 0 0 88 12 C
AM 0 0 88 12 C
AO 0 0 100 0 C
AP 0 0 88 12 C
AR 25 0 50 25 C
AU 25 0 50 25 C
AW 0 0 88 12 C
AX 0 0 88 12 C
AB 18 82 0 0 B
AC 21 79 0 0 B
K 67 33 0 0 B
L 0 100 0 0 B
N 0 100 0 0 B
P 0 100 0 0 B
U 67 33 0 0 B
V 67 33 0 0 B
X 67 33 0 0 B
Z 18 82 0 0 B
AD 0 100 0 0 B
Q 0 100 0 0 B
S 0 100 0 0 B
Y 21 79 0 0 B
A 67 33 0 0 A
B 67 33 0 0 A
C 67 33 0 0 A
D 67 33 0 0 A
E 63 37 0 0 A
F 25 0 50 25 A
G 67 33 0 0 A
H 67 33 0 0 A
I 67 33 0 0 A
J 21 79 0 0 A
AZ 0 0 0 100 D
BA_rot 0 0 0 100 D
BB 0 0 0 100 D
BC 0 0 0 100 D
BD 0 0 0 100 D
BG 0 0 0 100 D
BI 0 0 0 100 D
BK 0 0 0 100 D
NM1 0 0 88 12 D
NM2 25 0 50 25 D
BE 0 0 0 100 D
BF 0 0 0 100 D
BH 0 0 0 100 D
BJ 0 0 0 100 D
% probability
100
75
50
25
0
10. 10th Place

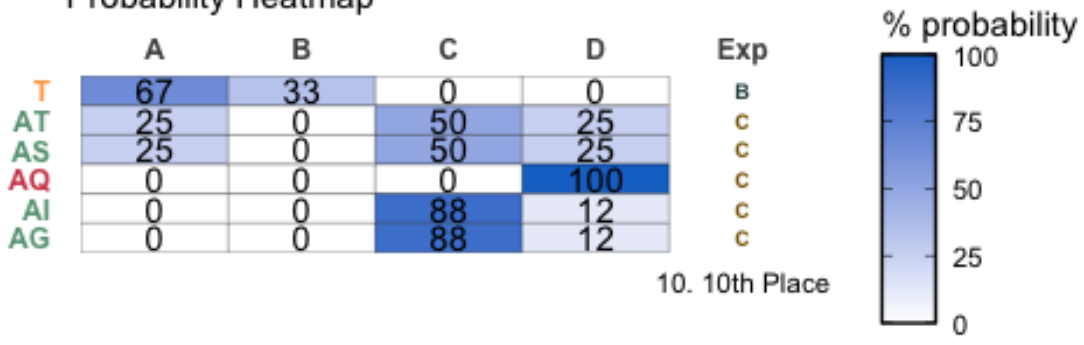

Test Set
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (33.3%)
2 (66.7%)
0 (0%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
3 (100%)
0 (0%)
3 (50%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
2 (100%)
3 (100%)
0 (0%)
6 (83.3%)
A
B
C
D
total
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True
10. 10th Place

Test Set

Probability Heatmap




External Validation
Confusion Matrix
A
B
C
D
total
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (100%)
0 (0%)
0 (0%)
0 (0%)
1 (16.7%)
0 (0%)
0 (0%)
4 (80%)
1 (20%)
5 (83.3%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
0 (0%)
1 (0%)
0 (0%)
4 (100%)
1 (0%)
6 (66.7%)
A
B
C
D
total
10. 10th Place
Proportion
0
25
50
75
100
Legend
Accuracy
False
Precision
Size
True

External Validation

Probability Heatmap