

CH Activation - 3-class - Top-10 Models

Section Results Summary

	Training.Accuracy	Test.Accuracy
1. 1st Place	94.44	90
2. 2nd Place	91.67	90
3. 3rd Place	91.67	90
4. 4th Place	91.67	90
5. 5th Place	91.67	90
6. 6th Place	91.67	60
7. 7th Place	86.11	90
8. 8th Place	86.11	90
9. 9th Place	86.11	90
10. 10th Place	86.11	90

Model Search

formula	McFadden R2
class ~ fr_amide + fr_para_hydroxylation + fr_pyridine	0.857
class ~ fr_C_O + fr_amide + fr_pyridine	0.818
class ~ fr_C_O_noCOO + fr_aldehyde + fr_pyridine	0.813
class ~ fr_C_O_noCOO + fr_amide + fr_pyridine	0.813
class ~ fr_aldehyde + fr_amide + fr_pyridine	0.813
class ~ fr_amide + fr_halogen + fr_pyridine	0.787
class ~ fr_Ar_N + fr_C_O_noCOO + fr_aldehyde	0.775
class ~ fr_Ar_N + fr_C_O_noCOO + fr_amide	0.775
class ~ fr_Ar_N + fr_aldehyde + fr_amide	0.775
class ~ fr_Ar_N + fr_C_O + fr_aldehyde	0.765

1st Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
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accuracy_formatted	McFadden_R2
94.44%	0.857

Model Coefficients

	(Intercept)	fr_ami de1	fr_ami de2	fr_para_hydroxylation1	fr_para_hydroxylation2	fr_pyridine1	fr_pyridine2
2	25.114767	2.505307	-14.50688	62.47374	-14.50688	-49.96827	7.804805
3	9.219008	20.598290	19.20727	77.27087	19.20727	-61.53297	-3.779301

Training Set

1	8 (100%)	0 (0%)	0 (0%)	8 (22%)
2	0 (0%)	13 (93%)	1 (7%)	14 (39%)
3	0 (0%)	1 (7%)	13 (93%)	14 (39%)
total	8 (100%)	14 (93%)	14 (93%)	36 (94%)
	1	2	3	total

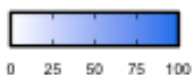
■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

1. 1st Place

Training Set

Probability Heatmap

	1	2	3	Exp
A	100	0	0	1
AB	0	75	25	2
AC	0	100	0	2
AD	0	100	0	2
AF	0	0	100	3
AG	0	10	90	3
AI	0	10	90	3
AL	0	10	90	3
AO	0	0	100	3
AP	0	10	90	3
AQ	0	75	25	3
AR	0	10	90	3
AS	0	10	90	3
AT	0	10	90	3
AU	0	10	90	3
AV	0	0	100	3
AW	0	10	90	3
AX	0	0	100	3
B	100	0	0	1
C	100	0	0	1
E	100	0	0	1
F	100	0	0	1
G	100	0	0	1
H	100	0	0	1
I	100	0	0	1
K	0	75	25	2
P	0	100	0	2
Q	0	100	0	2
S	0	10	90	2
T	0	100	0	2
U	0	100	0	2
V	0	100	0	2
W	0	100	0	2
X	0	100	0	2
Y	0	75	25	2
Z	0	100	0	2



1. 1st Place

Test Set

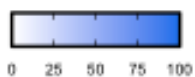
1	1 (50%)	1 (50%)	0 (0%)	2 (20%)
2	0 (0%)	4 (100%)	0 (0%)	4 (40%)
3	0 (0%)	0 (0%)	4 (100%)	4 (40%)
total	1 (100%)	5 (80%)	4 (100%)	10 (90%)
	1	2	3	total

■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

1. 1st Place

Test Set Probability Heatmap

	1	2	3	Exp
AH	0	10	90	3
AK	0	0	100	3
AM	0	0	100	3
AN	0	0	100	3
D	100	0	0	1
J	0	100	0	1
L	0	100	0	2
M	0	100	0	2
N	0	100	0	2
O	0	100	0	2



1. 1st Place

2nd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
91.67%	0.818

Model Coefficients

	(Intercept)	fr_C_O1	fr_C_O2	fr_amide 1	fr_amide 2	fr_pyridine1	fr_pyridine2
2	34.70423	-	47.48905	-	-	-35.80282	12.21598
		18.15717		33.95879	26.68061		
3	33.31792	-	-	21.01966	32.94425	-61.99185	-6.29827
		39.50878	38.51480				

Training Set

1	8 (100%)	0 (0%)	0 (0%)	8 (22%)
2	2 (14%)	12 (86%)	0 (0%)	14 (39%)
3	0 (0%)	1 (7%)	13 (93%)	14 (39%)
total	10 (80%)	13 (92%)	13 (100%)	36 (92%)
	1	2	3	total

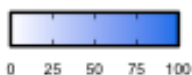
■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

2. 2nd Place

Training Set

Probability Heatmap

	1	2	3	Exp
A	75	25	0	1
AB	0	100	0	2
AC	0	100	0	2
AD	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3
AI	0	0	100	3
AL	0	0	100	3
AO	0	0	100	3
AP	0	0	100	3
AQ	0	80	20	3
AR	0	0	100	3
AS	0	0	100	3
AT	0	0	100	3
AU	0	0	100	3
AV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3
B	75	25	0	1
C	75	25	0	1
E	100	0	0	1
F	100	0	0	1
G	75	25	0	1
H	75	25	0	1
I	75	25	0	1
K	0	80	20	2
P	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
T	0	100	0	2
U	75	25	0	2
V	75	25	0	2
W	0	80	20	2
X	0	80	20	2
Y	0	80	20	2
Z	0	100	0	2



2. 2nd Place

Test Set

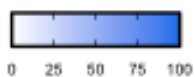
1	1 (50%)	1 (50%)	0 (0%)	2 (20%)
2	0 (0%)	4 (100%)	0 (0%)	4 (40%)
3	0 (0%)	0 (0%)	4 (100%)	4 (40%)
total	1 (100%)	5 (80%)	4 (100%)	10 (90%)
	1	2	3	total

■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

2. 2nd Place

Test Set Probability Heatmap

	1	2	3	Exp
AH	0	0	100	3
AK	0	0	100	3
AM	0	0	100	3
AN	0	0	100	3
D	75	25	0	1
J	0	80	20	1
L	0	100	0	2
M	0	100	0	2
N	0	100	0	2
O	0	100	0	2



2. 2nd Place

3rd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
91.67%	0.813

Model Coefficients

	(Intercept)	fr_C_O_noC OO1	fr_C_O_noC OO2	fr_aldehyde 1	fr_pyridine1	fr_pyridine2
2	79.07284	-57.48071	5.840504	14.19855	-80.17144	22.17891
3	77.46336	-36.39885	-2.877371	-83.61802	-99.72212	-12.58823

Training Set

1	8 (100%)	0 (0%)	0 (0%)	8 (22%)
2	2 (14%)	12 (86%)	0 (0%)	14 (39%)
3	0 (0%)	1 (7%)	13 (93%)	14 (39%)
total	10 (80%)	13 (92%)	13 (100%)	36 (92%)
	1	2	3	total

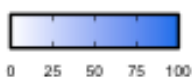
■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

3. 3rd Place

Training Set

Probability Heatmap

	1	2	3	Exp
A	75	25	0	1
AB	0	100	0	2
AC	0	100	0	2
AD	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3
AI	0	0	100	3
AL	0	0	100	3
AO	0	0	100	3
AP	0	0	100	3
AQ	0	83	17	3
AR	0	0	100	3
AS	0	0	100	3
AT	0	0	100	3
AU	0	0	100	3
AV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3
B	75	25	0	1
C	75	25	0	1
E	100	0	0	1
F	100	0	0	1
G	75	25	0	1
H	75	25	0	1
I	75	25	0	1
K	0	83	17	2
P	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
T	0	83	17	2
U	75	25	0	2
V	75	25	0	2
W	0	83	17	2
X	0	83	17	2
Y	0	83	17	2
Z	0	100	0	2



3. 3rd Place

Test Set

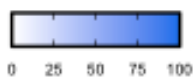
1	1 (50%)	1 (50%)	0 (0%)	2 (20%)
2	0 (0%)	4 (100%)	0 (0%)	4 (40%)
3	0 (0%)	0 (0%)	4 (100%)	4 (40%)
total	1 (100%)	5 (80%)	4 (100%)	10 (90%)
	1	2	3	total

■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

3. 3rd Place

Test Set Probability Heatmap

	1	2	3	Exp
AH	0	0	100	3
AK	0	0	100	3
AM	0	0	100	3
AN	0	0	100	3
D	75	25	0	1
J	0	83	17	1
L	0	100	0	2
M	0	100	0	2
N	0	100	0	2
O	0	100	0	2



3. 3rd Place

4th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
91.67%	0.813

Model Coefficients

	(Intercept)	fr_C_O_noC OO1	fr_C_O_noC OO2	fr_amid e1	fr_amid e2	fr_pyridine 1	fr_pyridine 2
2	34.46160	-17.23176	46.3166	- 33.5065 4	- 26.1448 6	-35.5602	11.352386
3	32.85215	-37.90227	-37.6383	19.8431 7	32.7142 5	-62.6160	-5.908221

Training Set

1	8 (100%)	0 (0%)	0 (0%)	8 (22%)
2	2 (14%)	12 (86%)	0 (0%)	14 (39%)
3	0 (0%)	1 (7%)	13 (93%)	14 (39%)
total	10 (80%)	13 (92%)	13 (100%)	36 (92%)
	1	2	3	total

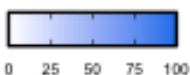
■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

4. 4th Place

Training Set

Probability Heatmap

	1	2	3	Exp
A	75	25	0	1
AB	0	100	0	2
AC	0	100	0	2
AD	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3
AI	0	0	100	3
AL	0	0	100	3
AO	0	0	100	3
AP	0	0	100	3
AQ	0	83	17	3
AR	0	0	100	3
AS	0	0	100	3
AT	0	0	100	3
AU	0	0	100	3
AV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3
B	75	25	0	1
C	75	25	0	1
E	100	0	0	1
F	100	0	0	1
G	75	25	0	1
H	75	25	0	1
I	75	25	0	1
K	0	83	17	2
P	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
T	0	83	17	2
U	75	25	0	2
V	75	25	0	2
W	0	83	17	2
X	0	83	17	2
Y	0	83	17	2
Z	0	100	0	2



4. 4th Place

Test Set

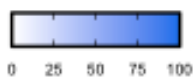
1	1 (50%)	1 (50%)	0 (0%)	2 (20%)
2	0 (0%)	4 (100%)	0 (0%)	4 (40%)
3	0 (0%)	0 (0%)	4 (100%)	4 (40%)
total	1 (100%)	5 (80%)	4 (100%)	10 (90%)
	1	2	3	total

■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

4. 4th Place

Test Set Probability Heatmap

	1	2	3	Exp
AH	0	0	100	3
AK	0	0	100	3
AM	0	0	100	3
AN	0	0	100	3
D	75	25	0	1
J	0	83	17	1
L	0	100	0	2
M	0	100	0	2
N	0	100	0	2
O	0	100	0	2



4. 4th Place

5th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
91.67%	0.813

Model Coefficients

	(Intercept)	fr_aldehyde1	fr_amide1	fr_amide2	fr_pyridine1	fr_pyridine2
2	46.67155	-22.67067	-8.248525	-24.18203	-47.77032	13.681589
3	45.06217	-55.57078	8.167943	32.15144	-63.79193	-8.620976

Training Set

1	8 (100%)	0 (0%)	0 (0%)	8 (22%)
2	2 (14%)	12 (86%)	0 (0%)	14 (39%)
3	0 (0%)	1 (7%)	13 (93%)	14 (39%)
total	10 (80%)	13 (92%)	13 (100%)	36 (92%)
	1	2	3	total

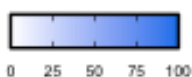
■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

5. 5th Place

Training Set

Probability Heatmap

	1	2	3	Exp
A	75	25	0	1
AB	0	100	0	2
AC	0	100	0	2
AD	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3
AI	0	0	100	3
AL	0	0	100	3
AO	0	0	100	3
AP	0	0	100	3
AQ	0	83	17	3
AR	0	0	100	3
AS	0	0	100	3
AT	0	0	100	3
AU	0	0	100	3
AV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3
B	75	25	0	1
C	75	25	0	1
E	100	0	0	1
F	100	0	0	1
G	75	25	0	1
H	75	25	0	1
I	75	25	0	1
K	0	83	17	2
P	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
T	0	83	17	2
U	75	25	0	2
V	75	25	0	2
W	0	83	17	2
X	0	83	17	2
Y	0	83	17	2
Z	0	100	0	2



Test Set

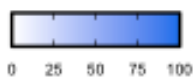
1	1 (50%)	1 (50%)	0 (0%)	2 (20%)
2	0 (0%)	4 (100%)	0 (0%)	4 (40%)
3	0 (0%)	0 (0%)	4 (100%)	4 (40%)
total	1 (100%)	5 (80%)	4 (100%)	10 (90%)
	1	2	3	total

■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

5. 5th Place

Test Set Probability Heatmap

	1	2	3	Exp
AH	0	0	100	3
AK	0	0	100	3
AM	0	0	100	3
AN	0	0	100	3
D	75	25	0	1
J	0	83	17	1
L	0	100	0	2
M	0	100	0	2
N	0	100	0	2
O	0	100	0	2



5. 5th Place

6th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
91.67%	0.787

Model Coefficients

	(Intercept)	fr_amide 1	fr_amid e2	fr_halogen 1	fr_halogen 3	fr_pyridine1	fr_pyridine2
2	29.85091	-	-	-17.16508	-6.314590	-31.10367	40.54860
		11.17984	24.9439				
		2	2				
3	11.75404	9.314921	33.4302	32.57566	8.089875	-38.20560	-34.52375
			7				

Training Set

1	8 (100%)	0 (0%)	0 (0%)	8 (22%)
2	2 (14%)	11 (79%)	1 (7%)	14 (39%)
3	0 (0%)	0 (0%)	14 (100%)	14 (39%)
total	10 (80%)	11 (100%)	15 (93%)	36 (92%)
	1	2	3	total

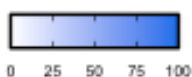
■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

6. 6th Place

Training Set

Probability Heatmap

	1	2	3	Exp
A	78	22	0	1
AB	0	100	0	2
AC	0	100	0	2
AD	0	100	0	2
AF	0	8	92	3
AG	0	8	92	3
AI	0	0	100	3
AL	0	8	92	3
AO	0	0	100	3
AP	0	8	92	3
AQ	0	0	100	3
AR	0	8	92	3
AS	0	8	92	3
AT	0	8	92	3
AU	0	8	92	3
AV	0	8	92	3
AW	0	8	92	3
AX	0	8	92	3
B	78	22	0	1
C	78	22	0	1
E	78	22	0	1
F	100	0	0	1
G	78	22	0	1
H	78	22	0	1
I	78	22	0	1
K	0	100	0	2
P	0	100	0	2
Q	0	100	0	2
S	0	8	92	2
T	0	100	0	2
U	78	22	0	2
V	78	22	0	2
W	0	100	0	2
X	0	100	0	2
Y	0	100	0	2
Z	0	100	0	2



Test Set

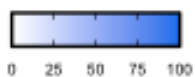
1	1 (50%)	1 (50%)	0 (0%)	2 (20%)
2	0 (0%)	1 (25%)	3 (75%)	4 (40%)
3	0 (0%)	0 (0%)	4 (100%)	4 (40%)
total	1 (100%)	2 (50%)	7 (57%)	10 (60%)
	1	2	3	total

■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

6. 6th Place

Test Set Probability Heatmap

	1	2	3	Exp
AH	0	8	92	3
AK	0	8	92	3
AM	0	8	92	3
AN	0	8	92	3
D	100	0	0	1
J	0	100	0	1
L	0	100	0	2
M	0	0	100	2
N	0	0	100	2
O	0	0	100	2



6. 6th Place

7th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
86.11%	0.775

Model Coefficients

	(Intercept)	fr_Ar_N1	fr_Ar_N2	fr_C_O_noCO O1	fr_C_O_noCO O2	fr_aldehyde1
2	41.71573	- 42.12124	1.385836	-30.869168	2.634101	10.27640
3	13.91867	- 34.53931	28.48981 8	9.569282	-1.282394	-47.03068

Training Set

1	8 (100%)	0 (0%)	0 (0%)	8 (22%)
2	4 (29%)	10 (71%)	0 (0%)	14 (39%)
3	0 (0%)	1 (7%)	13 (93%)	14 (39%)
total	12 (67%)	11 (91%)	13 (100%)	36 (86%)
	1	2	3	total

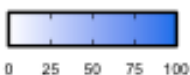
■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

7. 7th Place

Training Set

Probability Heatmap

	1	2	3	Exp
A	60	40	0	1
AB	0	100	0	2
AC	0	67	33	2
AD	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3
AI	0	0	100	3
AL	0	0	100	3
AO	0	0	100	3
AP	0	0	100	3
AQ	0	67	33	3
AR	0	0	100	3
AS	0	0	100	3
AT	0	0	100	3
AU	0	0	100	3
AV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3
B	60	40	0	1
C	60	40	0	1
E	100	0	0	1
F	100	0	0	1
G	60	40	0	1
H	60	40	0	1
I	60	40	0	1
K	0	100	0	2
P	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
T	60	40	0	2
U	60	40	0	2
V	60	40	0	2
W	0	100	0	2
X	60	40	0	2
Y	0	67	33	2
Z	0	100	0	2



Test Set

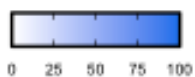
1	1 (50%)	1 (50%)	0 (0%)	2 (20%)
2	0 (0%)	4 (100%)	0 (0%)	4 (40%)
3	0 (0%)	0 (0%)	4 (100%)	4 (40%)
total	1 (100%)	5 (80%)	4 (100%)	10 (90%)
	1	2	3	total

■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

7. 7th Place

Test Set Probability Heatmap

	1	2	3	Exp
AH	0	0	100	3
AK	0	0	100	3
AM	0	0	100	3
AN	0	0	100	3
D	60	40	0	1
J	0	67	33	1
L	0	100	0	2
M	0	100	0	2
N	0	100	0	2
O	0	100	0	2



7. 7th Place

8th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
86.11%	0.775

Model Coefficients

	(Intercept)	fr_Ar_N1	fr_Ar_N 2	fr_C_O_noC OO1	fr_C_O_noC OO2	fr_amide 1	fr_amide 2
2	40.35748	-	3.7940	-17.59879	41.61749	-	-
		40.7629	3			39.7715	34.4431
		4				9	4
3	17.74330	-	25.715	-36.66409	-31.75876	35.3165	44.5734
		51.1476	07			9	5
		5					

Training Set

1	8 (100%)	0 (0%)	0 (0%)	8 (22%)
2	4 (29%)	10 (71%)	0 (0%)	14 (39%)
3	0 (0%)	1 (7%)	13 (93%)	14 (39%)
total	12 (67%)	11 (91%)	13 (100%)	36 (86%)
	1	2	3	total

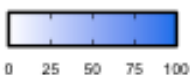
■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

8. 8th Place

Training Set

Probability Heatmap

	1	2	3	Exp
A	60	40	0	1
AB	0	100	0	2
AC	0	67	33	2
AD	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3
AI	0	0	100	3
AL	0	0	100	3
AO	0	0	100	3
AP	0	0	100	3
AQ	0	67	33	3
AR	0	0	100	3
AS	0	0	100	3
AT	0	0	100	3
AU	0	0	100	3
AV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3
B	60	40	0	1
C	60	40	0	1
E	100	0	0	1
F	100	0	0	1
G	60	40	0	1
H	60	40	0	1
I	60	40	0	1
K	0	100	0	2
P	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
T	60	40	0	2
U	60	40	0	2
V	60	40	0	2
W	0	100	0	2
X	60	40	0	2
Y	0	67	33	2
Z	0	100	0	2



Test Set

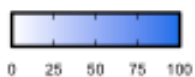
1	1 (50%)	1 (50%)	0 (0%)	2 (20%)
2	0 (0%)	4 (100%)	0 (0%)	4 (40%)
3	0 (0%)	0 (0%)	4 (100%)	4 (40%)
total	1 (100%)	5 (80%)	4 (100%)	10 (90%)
	1	2	3	total

■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

8. 8th Place

Test Set Probability Heatmap

	1	2	3	Exp
AH	0	0	100	3
AK	0	0	100	3
AM	0	0	100	3
AN	0	0	100	3
D	60	40	0	1
J	0	67	33	1
L	0	100	0	2
M	0	100	0	2
N	0	100	0	2
O	0	100	0	2



8. 8th Place

9th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
86.11%	0.775

Model Coefficients

	(Intercept)	fr_Ar_N1	fr_Ar_N2	fr_aldehyde1	fr_amide1	fr_amide2
2	40.46621	-40.87173	2.293119	-14.24134	-13.92313	-20.32962
3	18.46646	-48.99030	23.599784	-44.47311	20.37737	30.02969

Training Set

1	8 (100%)	0 (0%)	0 (0%)	8 (22%)
2	4 (29%)	10 (71%)	0 (0%)	14 (39%)
3	0 (0%)	1 (7%)	13 (93%)	14 (39%)
total	12 (67%)	11 (91%)	13 (100%)	36 (86%)
	1	2	3	total

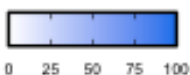
■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

9. 9th Place

Training Set

Probability Heatmap

	1	2	3	Exp
A	60	40	0	1
AB	0	100	0	2
AC	0	67	33	2
AD	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3
AI	0	0	100	3
AL	0	0	100	3
AO	0	0	100	3
AP	0	0	100	3
AQ	0	67	33	3
AR	0	0	100	3
AS	0	0	100	3
AT	0	0	100	3
AU	0	0	100	3
AV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3
B	60	40	0	1
C	60	40	0	1
E	100	0	0	1
F	100	0	0	1
G	60	40	0	1
H	60	40	0	1
I	60	40	0	1
K	0	100	0	2
P	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
T	60	40	0	2
U	60	40	0	2
V	60	40	0	2
W	0	100	0	2
X	60	40	0	2
Y	0	67	33	2
Z	0	100	0	2



Test Set

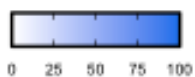
1	1 (50%)	1 (50%)	0 (0%)	2 (20%)
2	0 (0%)	4 (100%)	0 (0%)	4 (40%)
3	0 (0%)	0 (0%)	4 (100%)	4 (40%)
total	1 (100%)	5 (80%)	4 (100%)	10 (90%)
	1	2	3	total

■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

9. 9th Place

Test Set Probability Heatmap

	1	2	3	Exp
AH	0	0	100	3
AK	0	0	100	3
AM	0	0	100	3
AN	0	0	100	3
D	60	40	0	1
J	0	67	33	1
L	0	100	0	2
M	0	100	0	2
N	0	100	0	2
O	0	100	0	2



9. 9th Place

10th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
86.11%	0.765

Model Coefficients

	(Intercept)	fr_Ar_N1	fr_Ar_N2	fr_C_O1	fr_C_O2	fr_aldehyde1
2	24.84621	-25.53938	5.808112	0.6930752	4.278581	-11.01573
3	12.39437	-49.56023	17.566804	27.1056357	-1.104804	-56.78177

Training Set

1	8 (100%)	0 (0%)	0 (0%)	8 (22%)
2	4 (29%)	10 (71%)	0 (0%)	14 (39%)
3	0 (0%)	1 (7%)	13 (93%)	14 (39%)
total	12 (67%)	11 (91%)	13 (100%)	36 (86%)
	1	2	3	total

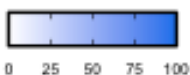
■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

10. 10th Place

Training Set

Probability Heatmap

	1	2	3	Exp
A	67	33	0	1
AB	0	100	0	2
AC	0	67	33	2
AD	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3
AI	0	0	100	3
AL	0	0	100	3
AO	0	0	100	3
AP	0	0	100	3
AQ	0	67	33	3
AR	0	0	100	3
AS	0	0	100	3
AT	0	0	100	3
AU	0	0	100	3
AV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3
B	67	33	0	1
C	67	33	0	1
E	100	0	0	1
F	50	50	0	1
G	67	33	0	1
H	67	33	0	1
I	67	33	0	1
K	0	100	0	2
P	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
T	50	50	0	2
U	67	33	0	2
V	67	33	0	2
W	0	100	0	2
X	67	33	0	2
Y	0	67	33	2
Z	0	100	0	2



Test Set

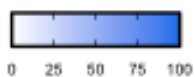
1	1 (50%)	1 (50%)	0 (0%)	2 (20%)
2	0 (0%)	4 (100%)	0 (0%)	4 (40%)
3	0 (0%)	0 (0%)	4 (100%)	4 (40%)
total	1 (100%)	5 (80%)	4 (100%)	10 (90%)
	1	2	3	total

■ Accuracy
 ■ False
 ■ Precision
 ■ Size
 ■ True

10. 10th Place

Test Set Probability Heatmap

	1	2	3	Exp
AH	0	0	100	3
AK	0	0	100	3
AM	0	0	100	3
AN	0	0	100	3
D	67	33	0	1
J	0	67	33	1
L	0	100	0	2
M	0	100	0	2
N	0	100	0	2
O	0	100	0	2



10. 10th Place