## 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

	McFadden
formula	R2
<pre>class ~ fr_amide + fr_para_hydroxylation + fr_pyridine</pre>	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

# accuracy\_formatted McFadden\_R2 94.44% 0.857

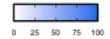
	(Interce	fr_ami	fr_ami	fr_para_hydroxyla	fr_para_hydroxyla	fr_pyridi	fr_pyridi
	pt)	de1	de2	tion1	tion2	ne1	ne2
2	25.1147	2.505	-	62.47374	-14.50688	-	7.80480
	67	307	14.50			49.9682	5
			688			7	
3	9.21900	20.59	19.20	77.27087	19.20727	-	-
	8	8290	727			61.5329	3.77930
						7	1

1	8	0	0	8	
	(100%)	(0%)	(0%)	(22%)	
2	0	13	1	14	
	(0%)	(93%)	(7%)	(39%)	
3	0	1	13	14	
	(0%)	(7%)	(93%)	(39%)	
total	8	14	14	36	
	(100%)	(93%)	(93%)	(94%)	
	1	2	3	total	
■ Accuracy ■ False ■ Precision ■ Size ■ True					

1. 1st Place

Training Set Probability Heatmap

		,		
	1	2	3	Exp
Α	100	0	0	1
AB	0	75	25	2
AC	0	100	0	2
AD	0	100	0	2 3 3 3 3 3
AF	0	0	100	3
AG	0	10	90	3
ΑI	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
ΑU	0	10	90	3
ΑV	0	0	100	3
AW	0	10	90	3
AX	0	0	100	3 3 3 3 3 3 3
В	100	0	0	1
C	100	0	0	1
Ε	100	0	0	1
F	100	0	0	1
G	100	0	0	1
Н	100	0	0	1
- 1	100	0	0	1
K	0	75	25	2
Р	0	100	0	2
Q	0	100	0	2
S	0	10	90	2
Т	0	100	0	2
T U	0	100	0	2
V	0	100	0	2
W	0	100	0	2
Х	0	100	0	2 2 2 2 2 2
Y Z	0	75	25	2
Z	0	100	0	2



1. 1st Place

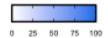
**Test Set** 

1	1	1	0	2	
	(50%)	(50%)	(0%)	(20%)	
2	0	4	0	4	
	(0%)	(100%)	(0%)	(40%)	
3	0	0	4	4	
	(0%)	(0%)	(100%)	(40%)	
total	1	5	4	10	
	(100%)	(80%)	(100%)	(90%)	
,	1	2	3	total	
■ Accuracy ■ False ■ Precision ■ Size ■ True					

1. 1st Place

Test Set Probability Heatmap

	1	2	3	Exp
АН	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
0	0	100	0	2



#### 2nd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy\_formatted McFadden\_R2 91.67% 0.818

				fr_amide	fr_amide		
	(Intercept)	fr_C_01	fr_C_02	1	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				

1	8	0	0	8	
	(100%)	(0%)	(0%)	(22%)	
2	2	12	0	14	
	(14%)	(86%)	(0%)	(39%)	
3	0	1	13	14	
	(0%)	(7%)	(93%)	(39%)	
total	10	13	13	36	
	(80%)	(92%)	(100%)	(92%)	
	1	2	3	total	
■ Accuracy ■ False ■ Precision ■ Size ■ True					
2	2nd Place				

2. 2nd Place

Training Set Probability Heatmap

		,		
	1	2	3	Exp
Α	75	25	0	1
AB	0	100	0	2
AC	0	100	0	2
AD	0	100	0	2 3 3 3 3 3
AF	0	0	100	3
AG	0	0	100	3
ΑI	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
ΑV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3 3 3 3 3 3 3
В	75	25	0	1
C	75	25	0	1
E	100	0	0	1
F	100 75 75	0	0	1
G	75	25	0	1
Н	75	25	0	1
- 1	75	25	0	1
K	0	80	20	2
Р	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
Т	0	100	0	2
T U	0 75	25	0	2
V	75	25	0	2
W	0	80	20	2 2 2 2 2 2
X	0	80	20	2
Y Z	0	80	20	2
Z	0	100	0	2



2. 2nd Place

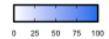
**Test Set** 

1	1	1	0	2	
	(50%)	(50%)	(0%)	(20%)	
2	0	4	0	4	
	(0%)	(100%)	(0%)	(40%)	
3	0	0	4	4	
	(0%)	(0%)	(100%)	(40%)	
total	1	5	4	10	
	(100%)	(80%)	(100%)	(90%)	
·	1	2	3	total	
■ Accuracy ■ False ■ Precision ■ Size ■ True					

2. 2nd Place

Test Set Probability Heatmap

	1	2	3	Exp
АН	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
0	0	100	0	2



#### 3rd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy\_formatted McFadden\_R2 91.67% 0.813

		fr_C_O_noC	fr_C_O_noC	fr_aldehyde		
	(Intercept)	001	002	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



3. 3rd Place

Training Set Probability Heatmap

	1	2	3	Exp
Α	75	25	0	1
AB	0	100	0	2
AC	0	100	0	
AD	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3 3 3 3 3 3 3
ΑI	0	0	100	3
AL	0	0	100	3
AO AP	0 0 0	0	100 100	3
AP	0	0	100	3
AQ AR	0	83	17 100	3
AR	0	0	100	3
AS AT	0	0	100	3
AT	0	0	100	3
ΑU	0	0	100	3
ΑV	0	0	100	3
AU AV AW	0	0	100 100	3
AX	0 0 <b>75</b>	0	100	3
B C E F G	75	25	0 0 0 0	3 3 3 1 1 1 1 1 1 2
C	75 100	25 0	0	1
E	100	0	0	1
F	100	0 25	0	1
G	75	25	0	1
H	75	25	0	1
- 1	100 75 75 75	25 25	0 17 0 0	1
K	0	83	17	2
K P	0 0 0	100	0	2
Q	0	100	0	2
S	0	100	0	2
Т	0	83	17	2
U	75	25	0	2
U V	75	25 25	0 0 17 17 17	2
W	0	83	17	2
Х	0	83	17	2
W X Y Z	0 75 75 0 0	83		2 2 2 2 2 2 2
Z	0	100	0	2



3. 3rd Place

**Test Set** 

1	1	1	0	2		
	(50%)	(50%)	(0%)	(20%)		
2	0	4	0	4		
	(0%)	(100%)	(0%)	(40%)		
3	0	0	4	4		
	(0%)	(0%)	(100%)	(40%)		
total	1	5	4	10		
	(100%)	(80%)	(100%)	(90%)		
,	1	2	3	total		
■ Accuracy ■ False ■ Precision ■ Size ■ True						

3. 3rd Place

Test Set Probability Heatmap

	1	2	3	Exp
АН	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
0	0	100	0	2

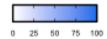


Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy\_formatted McFadden\_R2 91.67% 0.813

	(Intercept	fr_C_O_noC	fr_C_O_noC	fr_amid	fr_amid	fr_pyridine	fr_pyridine
	)	001	002	e1	e2	1	2
2	34.46160	-17.23176	46.3166	-	-	-35.5602	11.352386
				33.5065	26.1448		
				4	6		
3	32.85215	-37.90227	-37.6383	19.8431	32.7142	-62.6160	-5.908221
				7	5		

1	8	0	0	8			
	(100%)	(0%)	(0%)	(22%)			
2	2	12	0	14			
	(14%)	(86%)	(0%)	(39%)			
3	0	1	13	14			
	(0%)	(7%)	(93%)	(39%)			
total	10	13	13	36			
	(80%)	(92%)	(100%)	(92%)			
	1	2	3	total			
■ Accuracy ■ False ■ Precision ■ Size ■ True							
4	4. 4th Place						

Training Set Probability Heatmap

-				
	1	2	3	Exp
Α	75	25	0	1
AB	0	100	0	2
AC	0	100	0	2
AD AF	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3
ΑI	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		100	3
AS	0	0	100	3
AT	0	0	100	3
ΑU	0	0	100	3
ΑV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3
В	75	25	0	2 3 3 3 3 3 3 3 3 3 3 3 1
C	75	25	0	1
C E F G	100	0	0	1
F	100	0	0	1
G	100 75 75 75	25	0	1
н	75	25	0	1
- 1	75	25	0	1
K	0	83	17 0 0	2
P Q	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
Т	0	83	0	2
U	75	25	0	2
V	0 75 75	25 25	0	2
W	0	83	17	2
Х	0	83	17	2
W X Y Z	0	83	0 0 17 17 17	2 2 2 2 2 2
Z	0	100	0	2



4. 4th Place

**Test Set** 

1	1	1	0	2		
	(50%)	(50%)	(0%)	(20%)		
2	0	4	0	4		
	(0%)	(100%)	(0%)	(40%)		
3	0	0	4	4		
	(0%)	(0%)	(100%)	(40%)		
total	1	5	4	10		
	(100%)	(80%)	(100%)	(90%)		
	1	2	3	total		
■ Accuracy ■ False ■ Precision ■ Size ■ True						
4. 4th Place						

Test Set Probability Heatmap

	1	2	3	Exp
АН	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
0	0	100	0	2

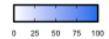
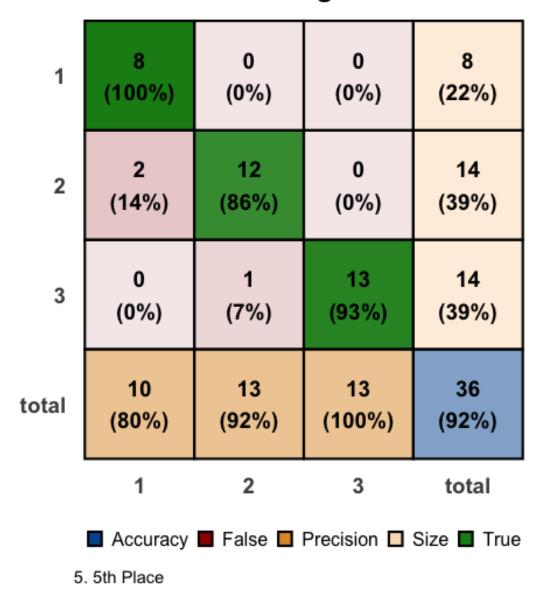


Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy\_formatted McFadden\_R2 91.67% 0.813

	(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 Probability Heatmap

	1	2	3	Exp
Α	75	25	0	1
AB	0	100	0	2
AC AD AF	0	100	0	2 2 3 3 3 3 3 3 3 3 3 3 3 1 1 1 1 1 1 2 2 2 2
AD	0	100	0	2
AF	0	0	100	3
AG	0	0	100	3
ΑI	0	0	100	3
AL	0	0	100	3
AO AP	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
ΑU	0	0	100	3
ΑV	0	0	100	3
AQ AR AS AT AU AV AW	0 0 75	0	100	3
AX	0	0	100	3
B C E F G	75	25	0	1
С	75 100	25 0 0	0	1
Ε	100	0	0	1
F	100	0	0	1
G	75	25	0	1
Н	75	25	0	1
H	100 75 75 75	25 25	0	1
K P	0 0 0	83 100	17 0 0 0	2
P	0	100	0	2
Q	0	100	0	2
S		100		2
Т	0	83	17	2
U	75 75	25 25	0	2
V	75	25	0	2
V W X Y	0 0 0	83	0 0 17 17 17	2 2 2 2 2 2 2 2
Х	0	83	17	2
Υ	0	83	17	2
Z	0	100	0	2



5. 5th Place

**Test Set** 

1	1	1	0	2		
	(50%)	(50%)	(0%)	(20%)		
2	0	4	0	4		
	(0%)	(100%)	(0%)	(40%)		
3	0	0	4	4		
	(0%)	(0%)	(100%)	(40%)		
total	1	5	4	10		
	(100%)	(80%)	(100%)	(90%)		
	1	2	3	total		
	■ Accuracy ■ False ■ Precision ■ Size ■ True					
5.	. 5th Place					

Test Set Probability Heatmap

	1	2	3	Exp
АН	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
0	0	100	0	2

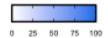
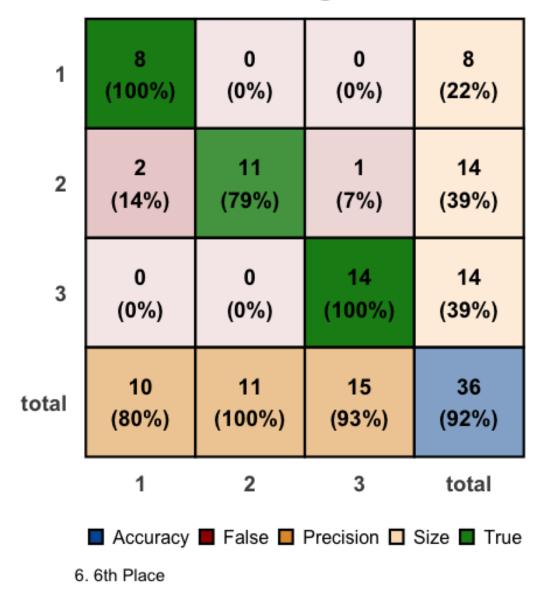


Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy\_formatted McFadden\_R2 91.67% 0.787

		fr_amide	fr_amid	fr_halogen	fr_halogen		
	(Intercept)	1	e2	1	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 Probability Heatmap

	r robability r roatmap				
	1	2	3	Exp	
Α	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	
ΑI	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	
ΑU	0	8	92	3	
AV	0	8	92	3	
AW	0	8	92	3	
AX	0	8	92	3	
В	78	22	0	3 3 3 3 3 3	
C	78	22 22	0	1	
E	78	22	0	1	
F	100	0	0	1	
G	78	22	0	1	
Н	78	22	0	1	
- 1	78	22	0	1	
K	0	100	0	2	
K P	0	100	0	2	
Q	0	100	0	2	
S	0	8	92	2	
Т	0	100	0	2	
T U	78	22	0	2	
V	78	22 22	0 0 0	2	
W	0	100	0	2	
Х	0	100	0	2 2 2 2 2 2 2	
W X Y Z	0	100	0	2	
Z	0	100	0	2	



6. 6th Place

**Test Set** 

1	1	1	0	2		
	(50%)	(50%)	(0%)	(20%)		
2	0	1	3	4		
	(0%)	(25%)	(75%)	(40%)		
3	0	0	4	4		
	(0%)	(0%)	(100%)	(40%)		
total	1	2	7	10		
	(100%)	(50%)	(57%)	(60%)		
	1	2	3	total		
■ Accuracy ■ False ■ Precision ■ Size ■ True						
6	6. 6th Place					

Test Set Probability Heatmap

	1	2	3	Exp
АН	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
М	0	0	100	2
N	0	0	100	2
0	0	0	100	2

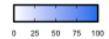


Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy\_formatted McFadden\_R2 86.11% 0.775

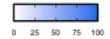
				fr_C_O_noCO	fr_C_O_noCO	
	(Intercept)	fr_Ar_N1	fr_Ar_N2	01	O2	fr_aldehyde1
2	41.71573	- 42.12124	1.385836	-30.869168	2.634101	10.27640
3	13.91867	- 34.53931	28.48981 8	9.569282	-1.282394	-47.03068

1	8	0	0	8
	(100%)	(0%)	(0%)	(22%)
2	4	10	0	14
	(29%)	(71%)	(0%)	(39%)
3	0	1	13	14
	(0%)	(7%)	(93%)	(39%)
total	12	11	13	36
	(67%)	(91%)	(100%)	(86%)
·	1	2	3	total
■ Accuracy ■ False ■ Precision ■ Size ■ True				
7.	7th Place			

7. 7th Place

Training Set Probability Heatmap

		,		
	1	2	3	Exp
Α	60	40	0	1
AB	0	100	0	2
AC	0	67	33	2
AD	0	100	0	2 3 3 3 3 3
AF	0	0	100	3
AG	0	0	100	3
ΑI	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
ΑU	0	0	100	3
ΑV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3
В	60	40	0	3 3 3 3 3 3 1 1
C	60	40	0	1
E	100	0	0	1
F	100	0	0	1
G	60	40	0	1
Н	60	40	0	1
- 1	60	40	0	1
K	0	100	0	2
P	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
	60	40	0	2
U	60	40	0	2
T U V	60	40	0	2
W	0	100	0	2
X	60	40		2 2 2 2 2 2
W X Y Z	0	67	33	2
Z	0	100	0	2



7. 7th Place

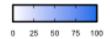
**Test Set** 

1	1	1	0	2		
	(50%)	(50%)	(0%)	(20%)		
2	0	4	0	4		
	(0%)	(100%)	(0%)	(40%)		
3	0	0	4	4		
	(0%)	(0%)	(100%)	(40%)		
total	1	5	4	10		
	(100%)	(80%)	(100%)	(90%)		
	1	2	3	total		
■ Accuracy ■ False ■ Precision ■ Size ■ True						
7	7. 7th Place					

7. 7th Place

Test Set Probability Heatmap

	1	2	3	Exp
АН	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
0	0	100	0	2
				-



### 8th Place

Table:

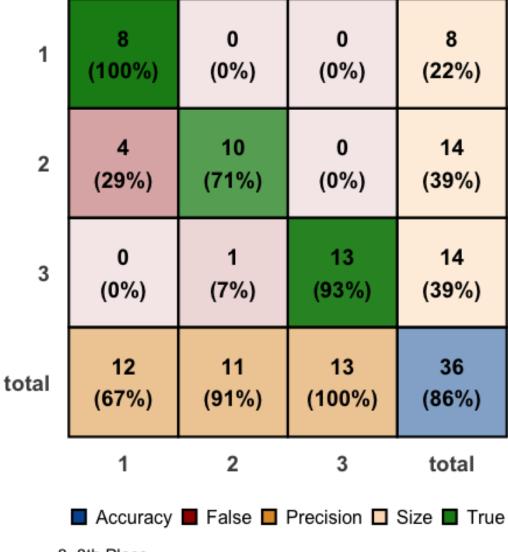
Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy\_formatted McFadden\_R2 86.11% 0.775

### **Model Coefficients**

			fr_Ar_N	fr_C_O_noC	fr_C_O_noC	fr_amide	fr_amide
	(Intercept)	fr_Ar_N1	2	001	002	1	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					

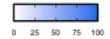
## **Training Set**



8. 8th Place

Training Set Probability Heatmap

riobability			Heat	Παρ
	1	2	3	Exp
Α	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
ΑI	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
ΑU	0	0	100	3
AV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	2 2 3 3 3 3 3 3 3 3 3 3 3 3 3 1 1
В	60	40	0	1
C	60	40	0	1
E F	100	0	0	1
	100	0	0	1
G	60	40	0	1
Н	60	40	0	1
- 1	60	40	0	1 2 2
K P	0	100	0	2
Р	0	100	0	
Q	0	100	0	2
S	0	100	0	2
T	60	40	0	2
T U V	60	40	0	2
V	60	40	0	2
W	0	100	0	2 2 2 2 2
W X Y Z	60	40	0	2
Υ	0	67	33	2
Z	0	100	0	2



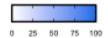
8. 8th Place

**Test Set** 

1	1	1	0	2			
	(50%)	(50%)	(0%)	(20%)			
2	0	4	0	4			
	(0%)	(100%)	(0%)	(40%)			
3	0	0	4	4			
	(0%)	(0%)	(100%)	(40%)			
total	1	5	4	10			
	(100%)	(80%)	(100%)	(90%)			
	1	2	3	total			
■ Accuracy ■ False ■ Precision ■ Size ■ True							
8	8. 8th Place						

Test Set Probability Heatmap

	1	2	3	Exp
АН	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
0	0	100	0	2



### 9th Place

Table:

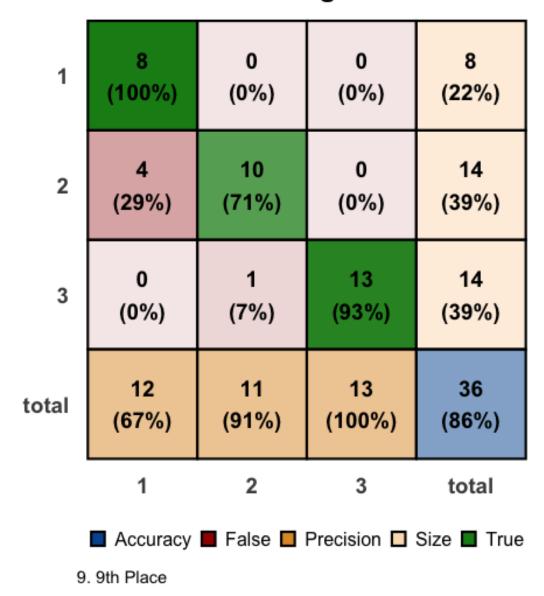
Full Model Stats - Overall Accuracy and Pseudo-R2

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**



Training Set Probability Heatmap

		,		
	1	2	3	Exp
Α	60	40	0	1
AB	0	100	0	2
AC	0	67	33	2
AD	0	100	0	2 3 3 3 3 3
AF	0	0	100	3
AG	0	0	100	3
ΑI	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
ΑV	0	0	100	3
AW	0	0	100	3
AX	0	0	100	3 3 3 3 3 3 3
В	60	40	0	1
C	60	40	0	1
E	100	0	0	1
F	100	0	0	1
G	60	40	0	1
Н	60	40	0	1
- 1	60	40	0	1
K	0	100	0	2
Р	0	100	0	2
Q	0	100	0	2
S	0	100	0	2
T	60	40	0	2
U	60	40	0	2
T U V	60	40	0	2
W	0	100	0	2
X	60	40	0	2 2 2 2 2 2
W X Y Z	0	67	33	2
Z	0	100	0	2

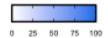
9. 9th Place

**Test Set** 

1	1	1	0	2	
	(50%)	(50%)	(0%)	(20%)	
2	0	4	0	4	
	(0%)	(100%)	(0%)	(40%)	
3	0	0	4	4	
	(0%)	(0%)	(100%)	(40%)	
total	1	5	4	10	
	(100%)	(80%)	(100%)	(90%)	
	1	2	3	total	
■ Accuracy ■ False ■ Precision ■ Size ■ True					
9	. 9th Place				

Test Set Probability Heatmap

	1	2	3	Exp
АН	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
0	0	100	0	2



### 10th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy\_formatted McFadden\_R2 86.11% 0.765

### **Model Coefficients**

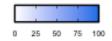
	(Intercept)	fr_Ar_N1	fr_Ar_N2	fr_C_O1	fr_C_O2	fr_aldehyde1
2	24.84621	-25.53938	5.808112	0.6930752	4.278581	-11.01573
3	12.39437	-49.56023	17.566804	27.1056357	-1.104804	-56.78177

# **Training Set**

1	8	0	0	8	
	(100%)	(0%)	(0%)	(22%)	
2	4	10	0	14	
	(29%)	(71%)	(0%)	(39%)	
3	0	1	13	14	
	(0%)	(7%)	(93%)	(39%)	
total	12	11	13	36	
	(67%)	(91%)	(100%)	(86%)	
·	1	2	3	total	
■ Accuracy ■ False ■ Precision ■ Size ■ True					
1	0. 10th Place				

### Training Set Probability Heatmap

	1	2	3	Exp
Α	67	33	0	1
AB	0	100	0	2
AC	0	67	33	2
AD	0	100	0	2
AF	0	0	100	3
AD AF AG	0	0	100	2 2 3 3 3 3 3 3 3 3 3 3 3 3 1 1 1 1 1 1
ΑI	0	0	100	3
AL	0	_ n	100 100	3
ΑO	0	0	100	3
AP	0	0	100	3
AQ	0	67	33	3
AR AS AT AU AV AW	0 0	0	100 100 33 100	3
AS	0	0	100	3
ΑT	0	0	100	3
ΑU	0	0	100	3
ΑV	0	0	100	3
ΑW	0	0	100	3
AX	0 0 0 67	0 0 0 33	100	3
	67	33	0	1
С	67	33	0	1
B C E F G H I	67 100	33 0 50	0	1
F	50 67	50	0	1
G	67	33	0	1
Н	67	33	0	1
- 1	67	33 33	0	1
K		100 100	0	2
K P Q S	0 0 0	100	0	2
Q	0	100	0	2
S	0	100	0	2
Т	50	50	0	2
U	67	33	0	2
V	67	33	0 0 0	2
W	0	100	0	2
X	0 67	33	0	2
V W X Y	0	33 67	33	2 2 2 2 2 2
Z	0	100	0	2



10. 10th Place

**Test Set** 

1	1	1	0	2				
	(50%)	(50%)	(0%)	(20%)				
2	0	4	0	4				
	(0%)	(100%)	(0%)	(40%)				
3	0	0	4	4				
	(0%)	(0%)	(100%)	(40%)				
total	1	5	4	10				
	(100%)	(80%)	(100%)	(90%)				
	1	2	3	total				
	■ Accuracy ■ False ■ Precision ■ Size ■ True							
1	0. 10th Place	10. 10th Place						

Test Set Probability Heatmap

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

