CH Activation - Binary Model - Top-10 Models - 3-features

Section Results Summary

	Training.Accuracy	Test.Accuracy
1. 1st Place	95.0	95
2. 2nd Place	87.5	80
3. 3rd Place	95.0	95
4. 4th Place	87.5	85
5.5th Place	87.5	95
6. 6th Place	92.5	95
7. 7th Place	82.5	65
8.8th Place	87.5	85
9. 9th Place	85.0	85
10. 10th Place	85.0	85

Model Search

formula	McFadden R2
class~fr_NH0+fr_NH1+fr_aldehyde	0.723
class~fr_Ar_N+fr_NH1+fr_aldehyde	0.540
class~fr_NH0+fr_aldehyde+fr_aniline	0.534
${\tt class \sim fr_C_0_noC00 + fr_NH0 + fr_piperdine}$	0.533
class~fr_Ar_N+fr_aldehyde+fr_amide	0.528
class~fr_NH0+fr_aldehyde+fr_amide	0.520
class~fr_NH0+fr_aldehyde+fr_piperdine	0.513
<pre>class ~ fr_Ar_N + fr_C_0_noCOO + fr_Imine</pre>	0.504
class~fr_Ar_N+fr_aldehyde+fr_aniline	0.504
<pre>class ~ fr_Ar_N + fr_C_0_noC00 + fr_aldehyde</pre>	0.491

1st Place

Table:

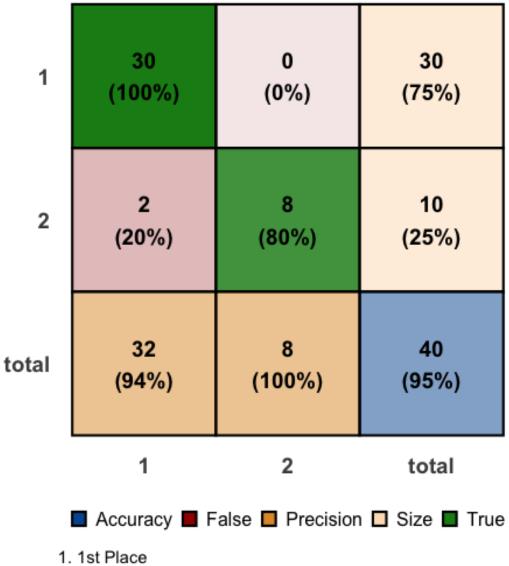
Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2

95%

0.723

	Х
(Intercept)	10.556389
fr_NH01	-13.041283
fr_NH02	-20.685858
fr_NH05	6.706012
fr_NH11	-12.165805
fr_NH12	-19.836949
fr aldehyde1	-22.331055

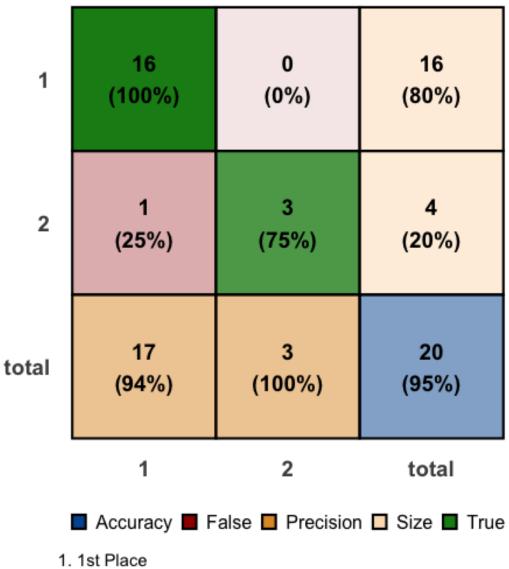


Training Set
Probability Heatmap

			,
	1	2	Exp
Α	92	8	1
B C D F G H	92	8	1
С	92	8	1
D	92 100	8	1
F	100	0	1
G	92	8	1
Н	92	8	1
AC	100	0	1
AD	100	0	1
K	92	8	1
L	100	0	1
M N	100	0	1
N	100	0	1
0	100	0	1
O P Q	100	0	1
Q	100	0	1
S	100	0	1
V	100 92		1
W	92	8	1
S V W X Y	92	8 0 0 17 17 17	111111111111111111111111111111111111111
Y	100	0	1
Z	100 100 83	0	1
AF	83	17	1
AK	83	17	1
AL AO AP	83	17	1
AO	100 83	0	1
AP	83	17	1
AR	92	8	1
AU	92	8	1
AW AZ	92 83	17	1
	. 0	17 100	2
BA_rot	0	100	2
BB	0	100	2
BC	0	100	2
BD	0	100	2
BG	0	100	2
BI	0	100	2
BK	0	100	2 2 2 2 2 2 2 2
NM1	83	17	2
NM2	92	8	2
	,		

0 25 50 75 100 1. 1st Place

Test Set



Test Set Probability Heatmap

	1	2	Exp
Е	100	0	1
-1	92	8	1
J	100	0	1
AB	100	0	1
U	92	8	1
АН	83	17	1
AM	83	17	1
AN	83	17	1
AV	92	8	1
АХ	83	17	1
BE	0	100	2
BF	0	100	2
вн	0	100	2
BJ	100	0	2
Т	92	8	1
AT	92	8	1
AS	92	8	1
AQ	100	0	1
AI	83	17	1
AG	83	17	1



1. 1st Place

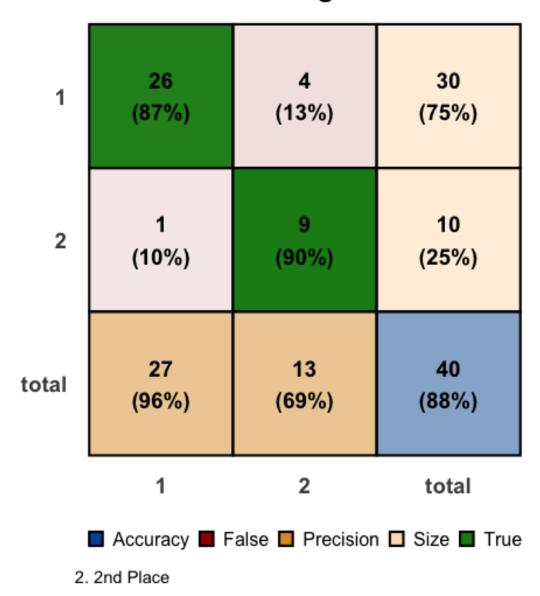
2nd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 87.5% 0.54

	Х
(Intercept)	0.6930372
fr_Ar_N1	-11.1760353
fr_Ar_N2	-12.3086573
fr_Ar_N3	8.0383966
fr_NH11	-2.3024413
fr_NH12	-11.7015089
fr_aldehyde1	-10.7895231

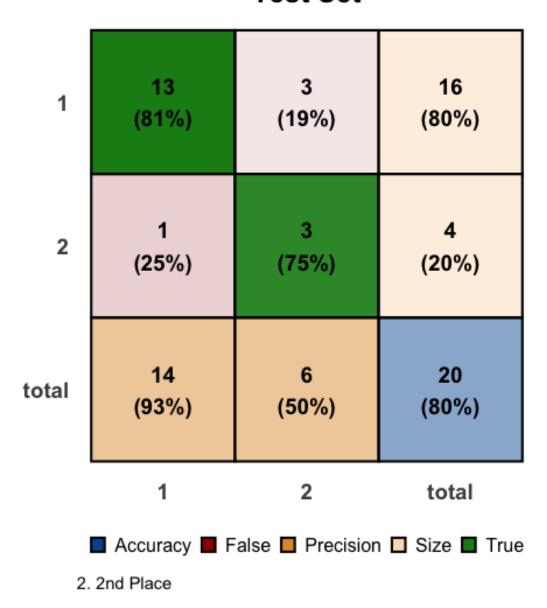


	1	2	Ехр
Α	100	0	1
В	100	0	1
С	100	0	1
D	100	0	1
D F	100	0	1
G	100	0	1
Н	100	0	1
AC	100	0	1
AD	100	0	1
K	33	0 67	1 1 1 1 1 1 1
K L	100	0	1
M	100	0	1
N	100	0	1 1 1
N O	100 100	0	1
Р	100	0	1
P Q	100	Ö	1
S	100	0	1
V	100 100	0	1 1 1
W	33	67	1
W X	100	0	1
Υ	100	0	1 1 1 1
Z AF	100	0	1
AF	83	17	1
AK	83	17	1
AL	83	0 17 17 17	1 1 1
AO	100	0	1
AP	100 83	0 17 67 67	1
AR	33	67	1
AU	33	67	1
AW	83	17	1
AR AU AW AZ BA_rot	33 33 83 33 33	17 67 67	1 1 2 2
BA_rot	33	67	2
BB	33	67	2
BC	33	67	2
BD	33	67	2
BG	33 33 33	67 67	2
BI	33	67	2
BK	0	100	2
NM1	83	17	2 2 2 2 2 2 2
NM2	33	67	2



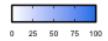
2. 2nd Place

Test Set



Test Set Probability Heatmap

	1	2	Exp
Е	100	0	1
- 1	100	0	1
J	100	0	1
AB	100	0	1
U	100	0	1
АН	83	17	1
ΑM	83	17	1
AN	83	17	1
AV	33	67	1
АХ	83	17	1
BE	33	67	2
BF	33	67	2
вн	33	67	2
BJ	100	0	2
Т	100	0	1
AT	33	67	1
AS	33	67	1
AQ	100	0	1
ΑI	83	17	1
AG	83	17	1



2. 2nd Place

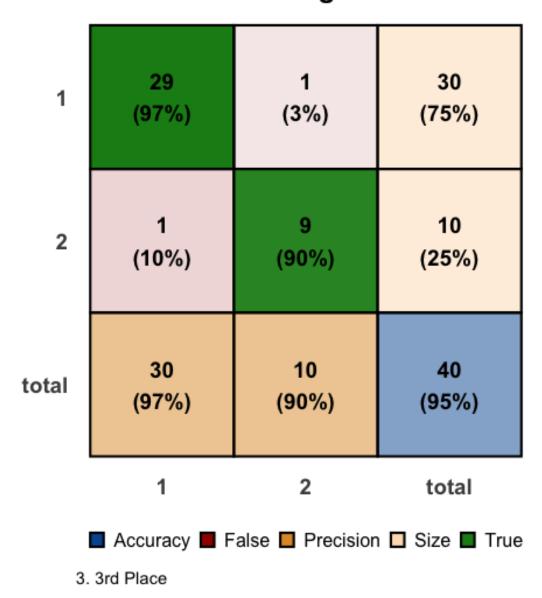
3rd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 95% 0.534

	X
(Intercept)	1.263219
fr_NH01	-3.679047
fr_NH02	-12.278576
fr_NH05	10.396818
fr_aldehyde1	-13.316024
fr_aniline1	-2.383742
fr aniline2	-11.709400



	1	2	Ехр
Α	92	8	1
В	92 92	8	1
С	92	8	1
D	92	8	1
B C D F G H	92 99 92 92	8 8 1 8 8 0 0	1
G	92	8	1
Н	92	8	1
AC	100 100 92 100 100 100	0	1
AD	100	0	1
K	92	8 0 0 0 0 0 0	1
L	100	0	1
M	100	0	1
N	100	0	1
0	100 100	0	1
Р	100 100	0	1
Q	100	0	1
S	100	0	1
V	92	8	1
W	92	8	1
X	92	8	1
Y	100	0	1
AD K L M N O P Q S V W X Y Z AF AK AL AO AP AR AU AW AZ BA rot	100 100 92 92 92 100 100 75 75 75 100 22 92 92 75 22 22	8 8 0 0 25 25 25 0 78 8 25 78 78	1
AF	75	25	1
AK	75	25	1
AL	75	25	1
AO	100	0	1
AP	22	78	1
AR	92	8	1
AU	92	8	1
AW	75	25	1
AZ	22	78	2
BA_rot	22	78	2
BB	22	78	2
BC	22	78 78	2
BD	22	78	2
BG	22	78	2
BI	22 22 22 22 22 22	78	2
BK	0	100	1111111111111111111111111112222222222
NM1	22	78	2
NM2	99	1	2
	,		



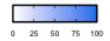
3. 3rd Place

Test Set



Test Set Probability Heatmap

	1	2	Exp
Е	100	0	1
-1	92	8	1
J	100	0	1
AB	100	0	1
U	92	8	1
АН	75	25	1
AM	75	25	1
AN	75	25	1
AV	99	1	1
AX	75	25	1
BE	22	78	2
BF	22	78	2
вн	22	78	2
BJ	100	0	2
Т	92	8	1
AT	92	8	1
AS	92	8	1
AQ	100	0	1
ΑI	75	25	1
AG	75	25	1



3. 3rd Place

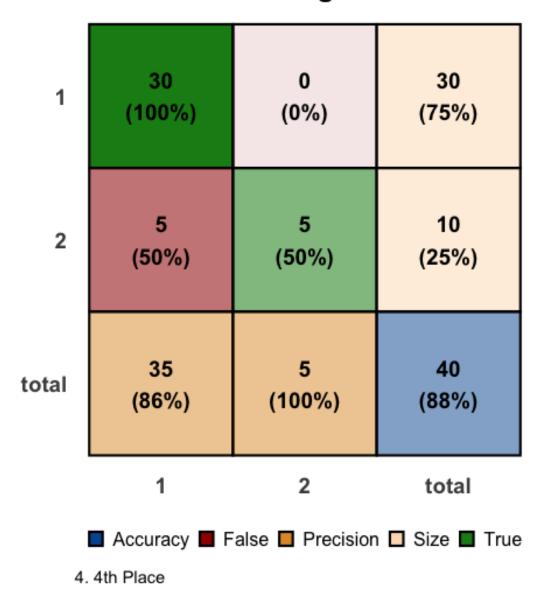
4th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 87.5% 0.533

	Х
(Intercept)	9.948232
fr_C_O_noCOO1	-11.414621
fr_C_O_noCOO2	-9.948442
fr_NH01	-20.378833
fr_NH02	-19.437518
fr_NH05	8.637000
fr_piperdine1	21.844837

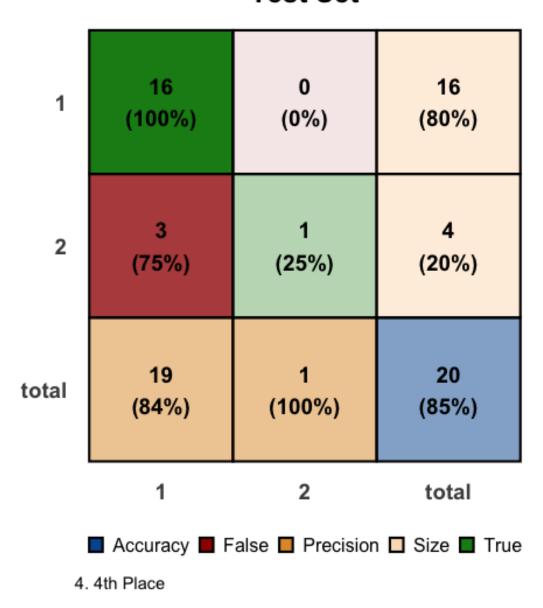


			,
	1	2	Ехр
Α	100	0	1
В	100	0	1
С	100	0	1
D F	100	0	1
F	100	0	1 1 1 1
G	100 100	Ω	1
Н	100	0	1
AC	100	0	1
AD	81	19	1 1 1
K	100 81	0	1
L	81	19	1
M N	81	19	1
N	81	19	1
O P Q	81	19 19 19 19	1
P	81	19	1 1 1
Q	81	19	1
S	50	50	1
V	100	0	1
W	100	0	1
S V W X Y	100 100	0 0	1 1 1 1
Y	100	0	1
Z	100	0 19 19 19	1 1 1
AF	81	19	1
AK	81	19	1
AL AO AP	81	19	1 1 1 1 1 2
AO	81	19	1
AP	81	19	1
AR	100 50	0	1
AU	50	50	1
AW AZ	81	19 100	1
AZ	0	100	2
BA_rot	81	19	2
BB	0	100	2
BC	0	100	2
BD	0	100	2
BG	81	19	2 2 2 2 2 2 2 2
BI	50	50	2
BK	0	100	2
NM1	81	19	2
NM2	50	50	2
	,		
		_	1

4.4th Place

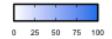
0 25 50 75 100

Test Set



Test Set Probability Heatmap

	1	2	Exp
Е	100	0	1
- 1	100	0	1
J	100	0	1
AB	100	0	1
U	100	0	1
АН	81	19	1
ΑM	81	19	1
AN	81	19	1
AV	100	0	1
АХ	81	19	1
BE	0	100	2
BE BF	0 81	100 19	2
BF	81	19	2
BF BH	81 81	19 19	2
BF BH BJ	81 81 100	19 19 0	2 2 2
BF BH BJ T	81 81 100 100	19 19 0 0	2 2 2 1
BF BH BJ T AT	81 81 100 100	19 19 0 0	2 2 2 1
BF BH BJ T AT	81 81 100 100 100	19 19 0 0 0	2 2 2 1 1
BF BH BJ T AT AS	81 100 100 100 100	19 19 0 0 0 0	2 2 1 1 1



4. 4th Place

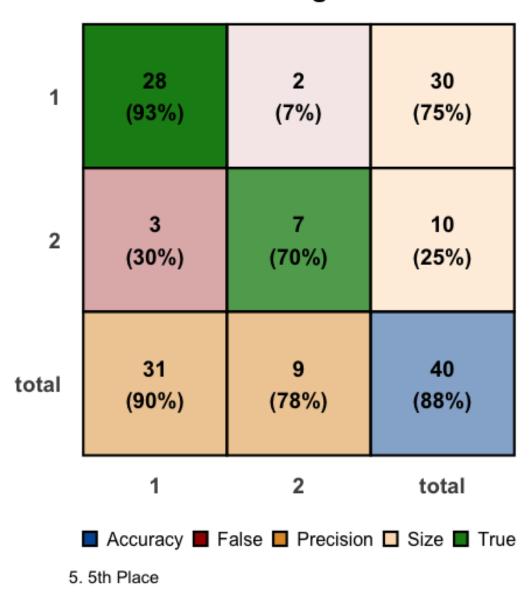
5th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 87.5% 0.528

	X
(Intercept)	1.098556
fr_Ar_N1	-17.532532
fr_Ar_N2	-13.087998
fr_Ar_N3	11.941262
fr_aldehyde1	-18.774855
fr_amide1	-1.945847
fr amide2	-12.438182

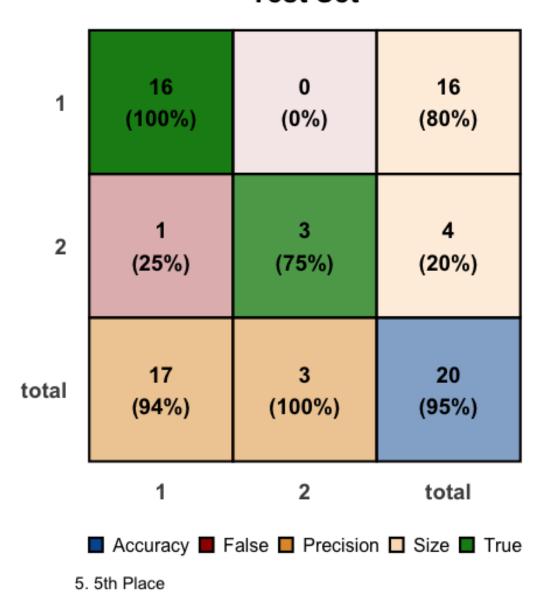


	1	2	Ехр
Α	100	0	1
В	100	0	1
С	100	0	1
D	100	0	1
D F	100	0	1
G	100	0	1
Н	100	0	1
AC	100	0	1
AD	100	0	1
K	25	75	1 1 1 1 1 1 1
K L	100		1
M	100	0	1
N	100	0	1 1 1
N O	100	0	1
P	100	0	1
P Q	100	ő	1
S	100	ő	1
v	100 100	0	1 1 1
w	25	75	i .
W X	100		1
Ŷ	100	0	1 1 1 1 1 1 1
7	100	0	1
Z AF	70	30	1
AK	70	30	1
AL	70	30	1
AO	100	0	1
AP	70	30	1
AR	70	30	1
ΔΙΙ	70	30	4
AU	70	30	4
AW AZ	100 70 70 70 100 70 70 70 70 25 25	30 30 30 30 75 75	1 1 2 2
BA_rot	25	75	2
BB	25	75	2
BC	25	75	2
BD		75 75	2
BG	25	30	2
BI	70 25	30 75	2
BK	0	100	2
NM1	70	30	2
NM2	70	30	2 2 2 2 2 2 2
NIVIZ	70	30	
	_		



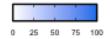
5. 5th Place

Test Set



Test Set Probability Heatmap

	1	2	Exp
Е	100	0	1
- 1	100	0	1
J	100	0	1
AB	100	0	1
U	100	0	1
АН	70	30	1
AM	70	30	1
AN	70	30	1
AV	70	30	1
АХ	70	30	1
BE	25	75	2
BF	25	75	2
вн	25	75	2
BJ	100	0	2
Т	100	0	1
АТ	70	30	1
AS	70	30	1
AQ	100	0	1
ΑI	70	30	1
AG	70	30	1



5. 5th Place

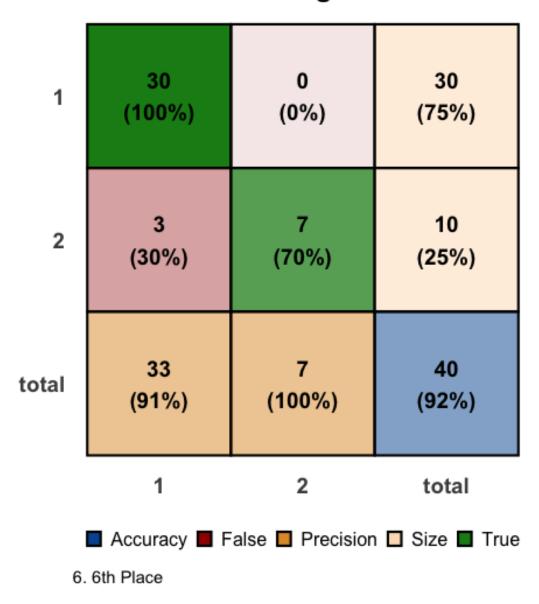
6th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 92.5% 0.52

	X
(Intercept)	1.677758
fr_NH01	-3.938551
fr_NH02	-12.268755
fr_NH05	9.909325
fr_aldehyde1	-14.535028
fr_amide1	-1.998048
fr_amide2	-11.605657

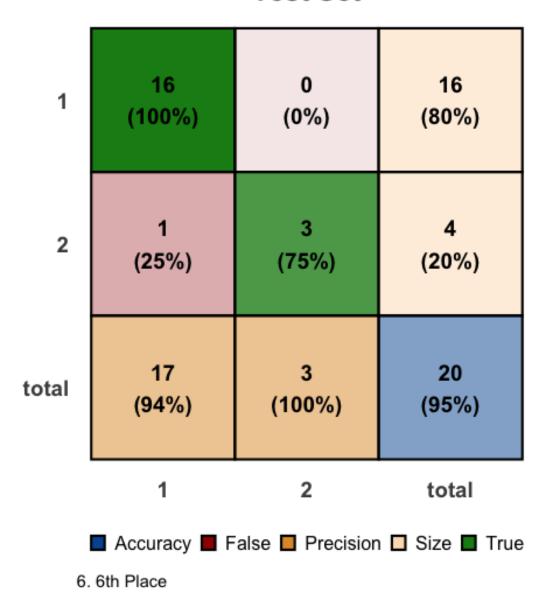


			,
	1	2	Ехр
Α	91	9	1
	91	9	1
С	91	9	1
D	91	9	1
B C D F G H	99	9 9 1 9 0 0 0 0 0 0 0	1
G	91	9	1
Н	91	9	1
AC	100	0	1
AD K	100 100 91 100 100	0	1
K	91	9	1
L	100	0	1
M	100	0	1
N	100	0	1
0	100	0	1
Р	100 100	0	1
Q	100	0	1
S	100	0	1
V	100 100 91	9	1
W	91	9	1
Х	91	9	1
L M NOPQSVWXYZ AFAK AOAPAR AUAW AZ	91 100 100 58 58 58	9 0 0 42 42 42	1
Z	100	0	1
AF	58	42	1
AK	58	42	1
AL	58	42	1
AO	100	0	1
AP	58	42	1
AR	99	1	1
AU	99	1	1
AW	58	42	1
AZ	16	84	2
BA_rot	100 58 99 99 58 16 16	0 42 1 1 42 84 84	2
BB	16	84	2
BC	16	84	2
BD	16	84	2
BG	58	42	2
BI	16	84	2
BK	0	100	1111111111111111111111111112222222222
NM1	58	42	2
NM2	99	1	2
	,	'	'
		-	1



6. 6th Place

Test Set



Test Set Probability Heatmap

	1	2	Exp
Е	100	0	1
-1	91	9	1
J	100	0	1
AB	100	0	1
U	91	9	1
АН	58	42	1
AM	58	42	1
AN	58	42	1
AV	99	1	1
АХ	58	42	1
BE	16	84	2
BF	16	84	2
вн	16	84	2
BJ	100	0	2
Т	91	9	1
AT	99	1	1
AS	99	1	1
AQ	100	0	1
AI	58	42	1
AG	58	42	1



6. 6th Place

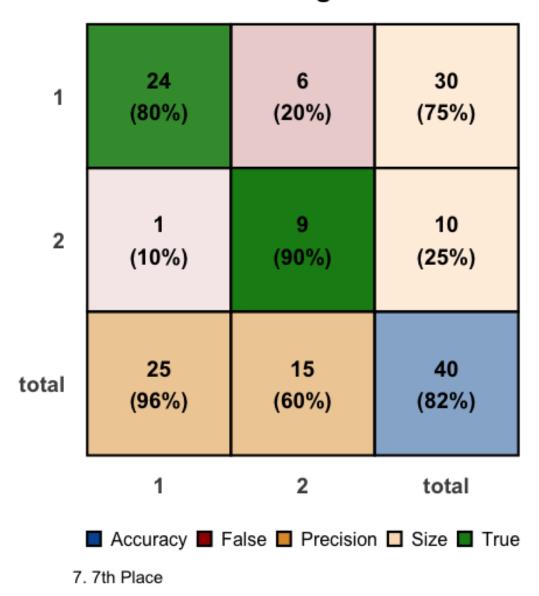
7th Place

Table:

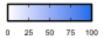
Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 82.5% 0.513

	X
(Intercept)	0.2876615
fr_NH01	-11.5717374
fr_NH02	-10.4352137
fr_NH05	9.4101726
fr_aldehyde1	-17.6542701
fr_piperdine1	11.2836406

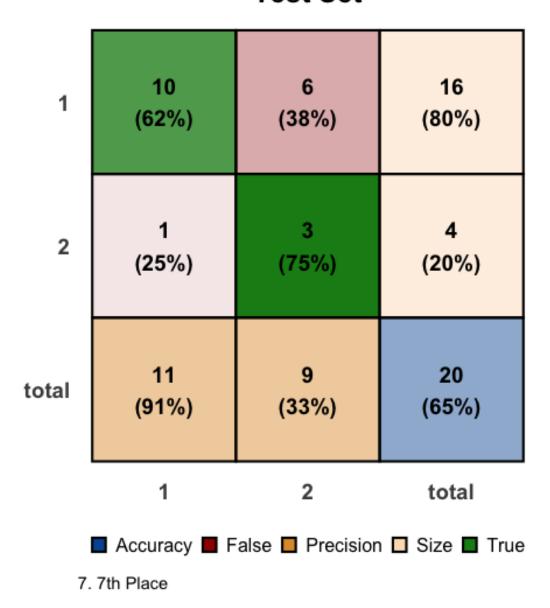


	1	2	Ехр
Α	100	0	1
B C D F G H	100	0	1
C	100	0	111111111111111111111111111111111111111
D	100	0	1
F	100	0	1
G	100	0	1
Н	100	0 0 0 0	1
AC	100 100	0	1
AD	100	0	1
K L M	100 100	0	1
L	100	0	1
M	100	0	1
N	100 100	0 0	1
0	100	0	1
P	100	0	1
Q	100	0	1
S	100	0 0	1
V	100	0	1
W	100	0	1
Х	100	0	1
Y	100 100	0	1
Z	100	0	1
N O P Q S V W X Y Z AF AK AL AO AP AR AU AW AZ BA_rot	43 43 43 43 100 50 43 43 43	0 0 0 57 57 57 57 57 57 57 57	1
AK	43	57	1
AL	43	57	1
AO	43	57	1
AP	43	57	1
AR	100	0	1
AU	50	50	1
AW	43	57	1
AZ	43	57	2
	43	57	
BB	43	57 57 57	2
BC	43	57	2
BD	43	57	2
BG	43 43 43	57	2
BI	43	57 57	2
BK	0	100 57	2
NM1	43	57	2 2 2 2 2 2 2
NM2	50	50	2
	_		_



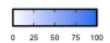
7. 7th Place

Test Set



Test Set Probability Heatmap

	1	2	Exp
Е	100	0	1
- 1	100	0	1
J	100	0	1
AB	100	0	1
U	100	0	1
АН	43	57	1
AM	43	57	1
AN	43	57	1
AV	100	0	1
AX	43	57	1
BE	43	57	2
BF	43	57	2
вн	43	57	2
BJ	100	0	2
Т	100	0	1
АТ	100	0	1
AS	100	0	1
AQ	100	0	1
Al	43	57	1
AG	43	57	1



7. 7th Place

8th Place

Table:

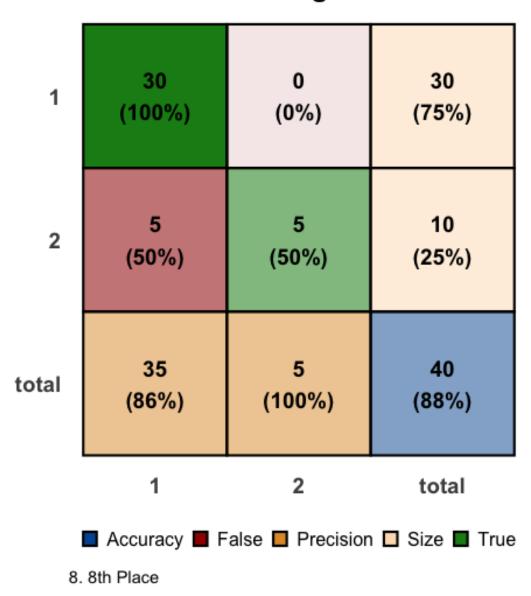
Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 87.5% 0.504

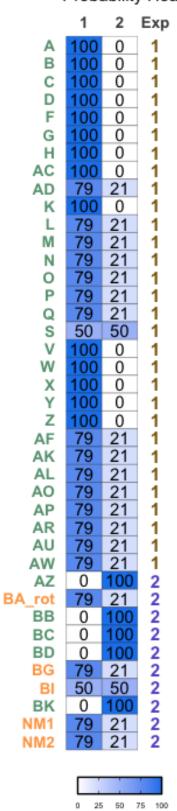
Model Coefficients

	Х
(Intercept)	9.947209
fr_Ar_N1	-20.699911
fr_Ar_N2	-19.316438
fr_Ar_N3	8.408516
fr_C_O_noCOO1	-11.268727
fr_C_O_noCOO2	-9.947352
fr_Imine1	-19.585137

Training Set

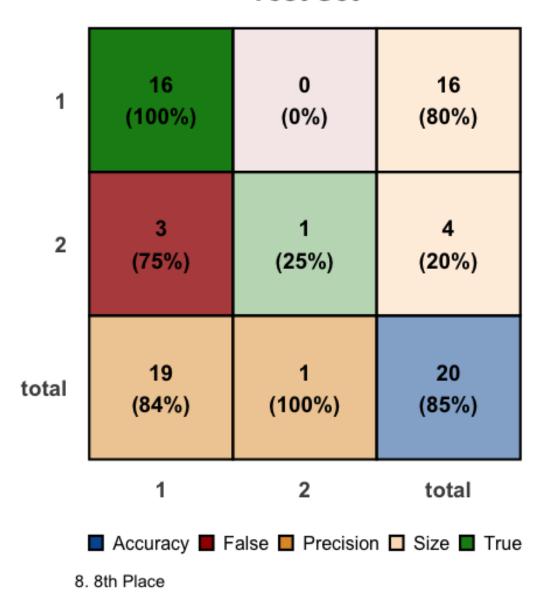


Training Set Probability Heatmap



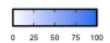
8.8th Place

Test Set



Test Set Probability Heatmap

	1	2	Exp
Е	100	0	1
- 1	100	0	1
J	100	0	1
AB	100	0	1
U	100	0	1
АН	79	21	1
AM	79	21	1
AN	79	21	1
AV	79	21	1
AX	79	21	1
BE	0	100	2
BE BF	0 79	100 21	
			2
BF	79	21	2
BF BH	79 79	21 21	2 2 2
BF BH BJ	79 79 100	21 21 0	2 2 2 2
BF BH BJ T	79 79 100 100	21 21 0	2 2 2 2 1
BF BH BJ T AT	79 79 100 100 79	21 21 0 0 21	2 2 2 2 1
BF BH BJ T AT	79 79 100 100 79 79	21 21 0 0 21 21	2 2 2 1 1
BF BH BJ T AT AS	79 79 100 100 79 79 100	21 21 0 0 21 21 0	2 2 2 1 1 1



8. 8th Place

9th Place

Table:

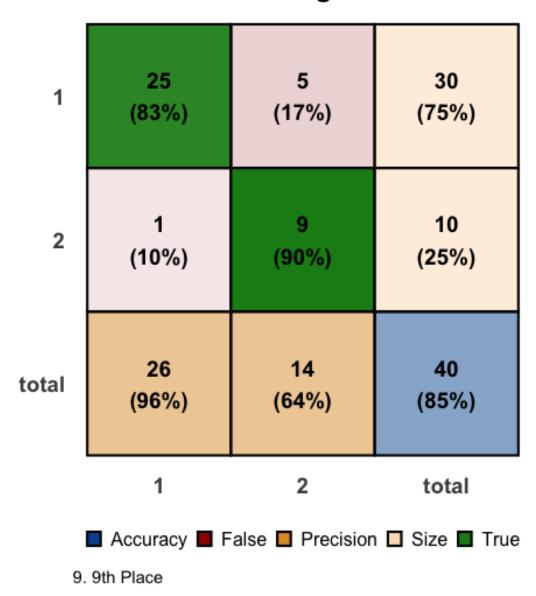
Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 85% 0.504

Model Coefficients

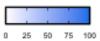
	X
(Intercept)	0.4698629
fr_Ar_N1	-10.9592651
fr_Ar_N2	-12.0477596
fr_Ar_N3	8.7230959
fr_aldehyde1	-10.5569212
fr_aniline1	-1.8560743
fr aniline2	-11.3290938

Training Set



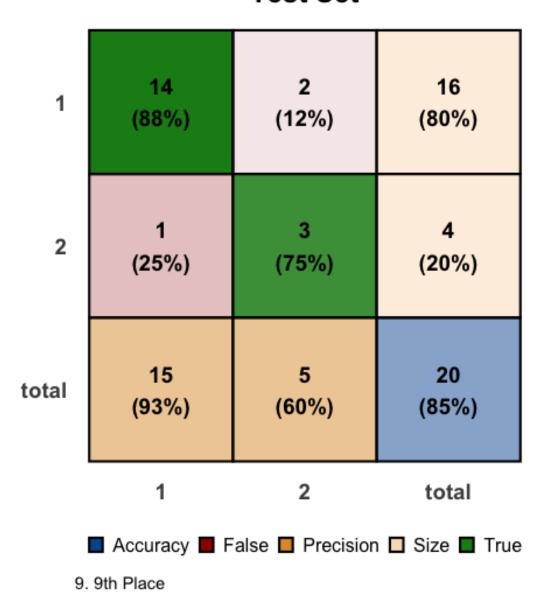
Training Set Probability Heatmap

	1	2	Ехр
Α	100	0	1
В	100	0	1
С	100	0	1
D	100	0	1
F	100	0	1
G	100		1
Н	100	0	1
AC	100	0	1
AD	100	0	1
K	38	62	1 1 1 1 1 1 1
K L	100	0	1
M	100	0	1
N	100	0	1 1 1
N O	100	0	1
Р	100	0	1
Q	100	0	1
S	100	0	1
V	100	0	1 1 1
W	38	62	1
W X	100	0	1
Y	100	0	1 1 1 1
Z AF	100	0	1
AF	80	20 20	1
AK	80	20	1
AL	80	20	1
AO	100	0	1 1 1
AP	38	0 62	1
AR	38	62	1
AU	38	62 62	1
AW	80	20	1
AW AZ	38 80 38 38	20 62 62	1 1 2 2
BA_rot	38	62	2
BB	38	62	2
BC	38	62	2
BD	38	62	2
BG	38	62	2
BI	38	62	2
BK	0	100	2
NM1	38	62	2 2 2 2 2 2 2
NM2	80	20	2



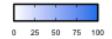
9. 9th Place

Test Set



Test Set Probability Heatmap

	1	2	Exp
Е	100	0	1
- 1	100	0	1
J	100	0	1
AB	100	0	1
U	100	0	1
АН	80	20	1
ΑM	80	20	1
AN	80	20	1
AV	80	20	1
АХ	80	20	1
BE	38	62	2
BF	38	62	2
вн	38	62	2
BJ	100	0	2
Т	100	0	1
AT	38	62	1
AS	38	62	1
AQ	100	0	1
ΑI	80	20	1
AG	80	20	1



10th Place

Table:

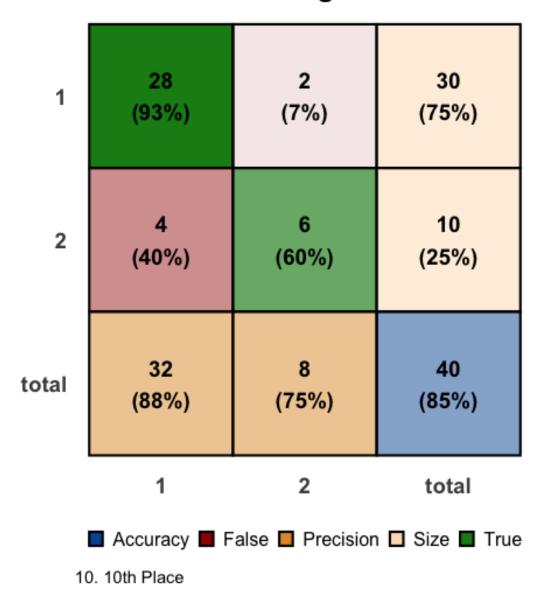
Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 85% 0.491

Model Coefficients

	Х
(Intercept)	0.6931781
fr_Ar_N1	-14.3266292
fr_Ar_N2	-16.5570786
fr_Ar_N3	10.1895186
fr_C_O_noCOO1	-1.3863029
fr_C_O_noCOO2	9.7573414
fr_aldehyde1	-23.9600787

Training Set



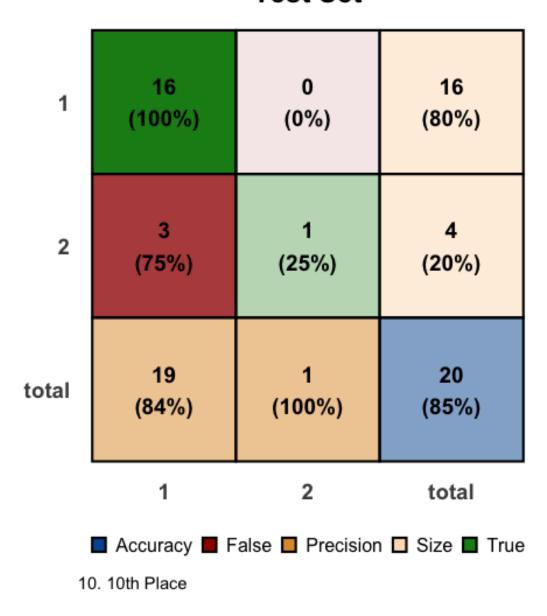
Training Set Probability Heatmap

	1	2	Exp
Α	100	0	1
В	100	0	1
C	100	0	1
D	100	0	1
F	100	0	1
F G H	100	0	1
Н	100	0	1
AC	100	0	1
AD	100	0	1
AC AD K L M N	33	0 67	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
L	100	0	1
M	100	0	1
N	100	0	1
0	100	0	1
P	100 100	0	1
Q	100	0	1
S	100 100	0	1
V	100	0	1
P Q S V W X	33	0 67	1
X	100	0 0 33 33 33 33 33 33 33 67	1
Y	100	0	1
Z	100	0	1 1 1 1 1 1 1 2
AF	67 67 67	33	1
AK	67	33	1
AL	67	33	1
AO	67	33	1
AO AP	67	33	1
AR	67	33	1
AU	67	33	1
AW	67	33	1
AZ	33	67	2
AW AZ BA_rot	67 67 67 67 67 33 67	33	2
BB	33 33	67 67	2
BC	33	67	2
BD	33	67	2
BG	67	33	2
BI	0	100	2
BK	0	100	2
NM1	67	33 33	2 2 2 2 2 2 2 2
NM2	67	33	2



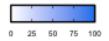
10. 10th Place

Test Set



Test Set Probability Heatmap

	1	2	Exp
Е	100	0	1
- 1	100	0	1
J	100	0	1
AB	100	0	1
U	100	0	1
АН	67	33	1
ΑM	67	33	1
AN	67	33	1
AV	67	33	1
АХ	67	33	1
BE	33	67	2
BF	67	33	2
вн	67	33	2
BJ	100	0	2
Т	100	0	1
АТ	67	33	1
AS	67	33	1
AQ	100	0	1
ΑI	67	33	1
AG	67	33	1



10. 10th Place