Pyridine Phosphination - 4-Feature Models - Non-ordinal

Section Results Summary

	Training.Accuracy	Test.Accuracy
1.1st Place	73.17	28.6
2. 2nd Place	80.49	28.6
3. 3rd Place	75.61	19.0
4. 4th Place	75.61	33.3
5. 5th Place	78.05	38.1
6. 6th Place	75.61	33.3
7.7th Place	68.29	42.9
8.8th Place	78.05	42.9
9. 9th Place	75.61	19.0
10. 10th Place	75.61	33.3

Model Search

formula	McFadden R2
class~L_1_SM+dip_y_SM+fr_halogen	0.647
class~NPA_1_P+dip_y_SM+fr_halogen	0.645
class $\sim loc.B5_1_SM + dip_y_SM + fr_halogen$	0.627
class~dip_y_P+dip_y_SM+fr_halogen	0.626
<pre>class ~ Total_P + fr_bicyclic + fr_halogen</pre>	0.624
class~NPA_4_P+dip_y_P+fr_halogen	0.619
$class \sim L_1_SM + dip_y_SM + fr_aryl_methyl$	0.610
class~Total_P+fr_ester+fr_halogen	0.608
class~NPA_7_SM+dip_y_SM+fr_halogen	0.607
class~dip_y_P+para_P+fr_halogen	0.605

1st Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2

73.17%

0.647

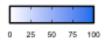
	(Interce		dip_y_	fr_halo	fr_halo	fr_halo	fr_halo	fr_halo	fr_halo
	pt)	L_1_SM	SM	gen1	gen2	gen3	gen4	gen5	gen6
2	-	0.41068	1.4979	-	121.62	211.54	-	-	204.26
	4.1394	05	02	0.8398	597	120	1.9513	130.82	026
	587			491			6	34	
3	724.20	-	-	-	102.62	-	-	171.07	-
	62843	111.882	90.919	97.099	806	64.020	12.110	83	62.925
		9913	791	8721		45	12		91
4	-	-	1.9500	1.9210	-	214.62	-	233.42	-
	0.8730	0.61251	88	199	38.629	140	124.40	69	25.127
	828	33			98		417		03

1	4	2	0	1	7
	(57%)	(29%)	(0%)	(14%)	(17%)
2	2	12	0	2	16
	(12%)	(75%)	(0%)	(12%)	(39%)
3	0	0	8	0	8
	(0%)	(0%)	(100%)	(0%)	(20%)
4	1	3	0	6	10
	(10%)	(30%)	(0%)	(60%)	(24%)
total	7	17	8	9	41
	(57%)	(71%)	(100%)	(67%)	(73%)
,	1	2	3	4	total
	■ Accura	cy I Fals	e 🔲 Precis	sion 🗖 Siz	e 🔳 True

1. 1st Place

Training Set Probability Heatmap

A 9 56 0 35 1 AF 18 12 0 70 1 B 68 31 0 1 C 48 50 0 3 D 82 18 0 0 1 E 86 14 0 0 1 F 69 30 0 2 AA 11 83 0 6 AB 1 81 0 18 2 AC 6 92 0 2 AH 46 11 0 44 2 AJ 0 89 0 11 G 17 83 0 0 2 J 10 74 0 16 K 0 32 0 68 M 26 67 0 8 2 T 14 74 0 11 U 0 100 0 0 2 X 18 82 0 0 2 AL 0 100 0 0 2 X 18 82 0 0 2 AL 0 100 0 0 3 AC 0 0 100 0 4 AC 0 67 0 33 AC 0 0 100 0 4 AC 0 67 0 33 AC 0 0 100 0 4 AC 0 67 0 33 AC 0 0 100 0 4 AC 0 67 0 33 AC 0 0 100 0 4 AC 0 67 0 33 AC 0 0 100 0 4 AC 0 67 0 33 AC 0 0 100 0 4 AC 0 67 0 33 AC 0 67 0 33 AC 0 0 100 0 4 AC 0 67 0 33 AC 0 67 0 30		1	2	3	4	Exp
AF	Α	9	56	0	35	1
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	AF	18	12	0	70	1
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	В	68	31	0	1	1
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	С	48	50	0	3	1
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	D	82	18	0	0	1
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	Е	86	14	0	0	1
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	F	69	30	0	2	1
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	AA	11	83	0	6	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	AB	1	81	0	18	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	AC	6	92	0	2	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	AH	46	11	0	44	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	AJ	0	89	0	11	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	G	17	83	0	0	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	J	10	74	0	16	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	K	0	32	0	68	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	M	26	67	0	8	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	Т	14	74	0	11	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	U	0	100	0	0	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	Х	18	82	0	0	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	AL	0	100	0	0	2
R 60 37 0 3 2 AO 0 0 100 0 3 AP 0 0 100 0 3 AQ 0 0 100 0 3 AR 0 0 100 0 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AT 0 0 100 0 3 AU 0 0 100 0 3 AN 0 0 100 0 3 AN 0 0 100 0 3 AW 0 40 0 60 4 AY 0 67 0 33 4 BA 0 11 0 89 4 BB 2 8 0 91 4 BB 2 8 0 91 4 BB 1 19 0 80 4	AM	30	64	0	6	2
AO	Н	0	40	0	60	2
BA 0 11 0 89 4 BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4	R	60	37	0	3	2
BA 0 11 0 89 4 BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4	AO	0	0	100	0	3
BA 0 11 0 89 4 BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4	AP	0	0	100	0	3
BA 0 11 0 89 4 BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4	AQ	0	0	100	0	3
BA 0 11 0 89 4 BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4	AR	0	0	100	0	3
BA 0 11 0 89 4 BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4	AS	0	0		0	3
BA 0 11 0 89 4 BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4	AT	0	0	100	0	3
BA 0 11 0 89 4 BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4	AU	0	0	100	0	3
BA 0 11 0 89 4 BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4	AN	0	0	100	0	3
BA 0 11 0 89 4 BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4	AW	0	40	0	60	4
BB 2 8 0 91 4 BC 7 56 0 37 4 BE 1 19 0 80 4 BH 0 0 0 100 4 BI 63 12 0 25 4 BJ 2 9 0 89 4			67	0	33	
BI 63 12 0 25 4 BJ 2 9 0 89 4		0		0	89	4
BI 63 12 0 25 4 BJ 2 9 0 89 4		2	8		91	4
BI 63 12 0 25 4 BJ 2 9 0 89 4		7	56		37	4
BI 63 12 0 25 4 BJ 2 9 0 89 4	BE	1	19	0	80	4
BJ 2 9 0 89 4 BK 8 56 0 36 4		0	0	0	100	4
BK 8 56 0 36 4	BI	63	12		25	4
BK 8 56 0 36 4		2	50		89	
	BK	8	56	U	36	4



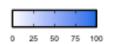
Test Set

1	0	0	0	0	0
	(0%)	(0%)	(0%)	(0%)	(0%)
2	2	5	5	3	15
	(13%)	(33%)	(33%)	(20%)	(71%)
3	0	0	0	0	0
	(0%)	(0%)	(0%)	(0%)	(0%)
4	1	2	2	1	6
	(17%)	(33%)	(33%)	(17%)	(29%)
total	3	7	7	4	21
	(0%)	(71%)	(0%)	(25%)	(29%)
	1	2	3	4	total
		_		-	

1. 1st Place

Test Set Probability Heatmap

	1	2	3	4	Exp
AD	0	90	0	10	2
AE	0	0	100	0	2
ΑI	15	56	0	29	2
AK	21	55	0	25	2
- 1	3	30	0	68	2
L	2	8	0	90	2
N	0	0	100	0	2
0	88	12	0	0	2
Р	0	0	100	0	2
Q	0	0	100	0	2
S	0	0	100	0	2
٧	11	81	0	8	2
W	3	96	0	0	2
Υ	45	34	0	21	2
Z	1	7	0	91	2
AV	0	0	100	0	4
AX	8	27	0	64	4
ΑZ	0	0	100	0	4
BD	21	54	0	25	4
BF	94	4	0	2	4
BG	0	100	0	0	4



2nd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 80.49% 0.645

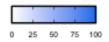
	(Interce	NPA_	dip_y	fr_halog	fr_halog	fr_halog	fr_halog	fr_halog	fr_halog
	pt)	1_P	_SM	en1	en2	en3	en4	en5	en6
2	-	1561.	23.65	-	194.488	298.800	-	-	242.171
	1341.50	944	436	4.11496	04	4	47.2432	138.194	62
	4			2			5	3	
3	-	1496.	20.52	-	190.854	-	-	264.310	-
	1281.24	313	290	5.09221	96	143.279	249.266	5	84.4482
	5			5		2	10		1
4	-	1567.	24.61	_	_	302.432	_	269.113	-
	1350.36	716	175	0.57759	39.5408	6	214.954	6	20.7042
	2			5	6		48		7

1	7	0	0	0	7
	(100%)	(0%)	(0%)	(0%)	(17%)
2	0	13	2	1	16
	(0%)	(81%)	(12%)	(6%)	(39%)
3	0	2	6	0	8
	(0%)	(25%)	(75%)	(0%)	(20%)
4	0	3	0	7	10
	(0%)	(30%)	(0%)	(70%)	(24%)
total	7	18	8	8	41
	(100%)	(72%)	(75%)	(88%)	(80%)
,	1	2	3	4	total
	■ Accura	cy I False	e 🔲 Precis	sion 🗖 Siz	e 🔳 True

2. 2nd Place

Training Set Probability Heatmap

	1	2	3	4	Exp
Α	100	0	0 1 0 0 0 2 0 8 0 2 38 0 4 5 0 28 24 0 0 17 30 0 85 58 37 84 99 83 76 15 61 0 0	0	1
AF	94	1	1	4	1
В	100	0	0	0	1
С	100	0	0	0	1
D	100 100 100	0	0	0	1
Ε	98	0	2	0	1
F	100	0	0	0	1
AA	0	80	8	13	2
AB	0	57	0	43	2
AC	0	82	2	16	2
AH	6	21	38	36	2
AJ	0	54	0	46	2
G	0	88	4	8	2
J	0	79	5	16	2
K	0	52	0	48	2
M	0	65	28	6	2
Т	2	66	24	9	2
U	0	100	0	0	2
Х	0	100	0	0	2
AL	0	83	17	0	2
BCDEFABCHAJGJKMTUXLMHROPQRSTUNWY	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 80 57 82 21 54 88 79 52 65 66 100 100 83 64 38 14 40 58 10 1 17 12 76 0 38 69	30	4 0 0 0 0 13 43 16 36 46 8 16 48 6 9 0 0 0 6 6 2 1 3 5 6 0 0 1 2 1 2 1 2 3 5 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	111111222222222222222333333344
Н	_0_	38	0	62	2
R	_0_	14	85	1_	2
AO	_0_	40	58	3	3
AP	0	58	37	-5	3
AQ	0	10	84	6	3
AR	0	1	99	0	3
AS	0	17	83	0	3
ΑT	0	12	76	12	3
ΑU	0	76	15	8	3
AN	0	0	61	39	3
AW	0	38	0	62	4
	0	69	0	31	
BA	_0_	25	0	75	4
BB	0	7	2	93	4
вс	0	77	2	93 21 96	4
BE	0	4	0	96	4
ВН	0	25 7 77 4 0 34	39	61	4
ВІ	0	34	2	64	4
BJ	0	9	0 39 2 0	61 64 91 22	4
BK	0	78	1	22	4



2. 2nd Place

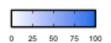
Test Set

1	0	0	0	0	0
	(0%)	(0%)	(0%)	(0%)	(0%)
2	3 (20%)	5 (33%)	1 (7%)	6 (40%)	15 (71%)
3	0	0	0	0	0
	(0%)	(0%)	(0%)	(0%)	(0%)
4	1	3	1	1	6
	(17%)	(50%)	(17%)	(17%)	(29%)
total	4	8	2	7	21
	(0%)	(62%)	(0%)	(14%)	(29%)
	1	2	3	4	total
	■ Accura	cy ■ Fals	e 🖪 Precis	sion 🗖 Siz	e 🔳 True

2. 2nd Place

Test Set Probability Heatmap

	1	2	3	4	Exp
AD	0	28	0	72	2
AE	0	49	46	4	2
ΑI	0	82	2	16	2
AK	0	79	10	11	2
-1	0	7	0	93	2
L	0	8	0	92	2
N	0	54	41	5	2
0	100	0	0	0	2
P	0	2	98	0	2
Q	100	0	0	0	2
S	100	0	0	0	2
٧	0	81	5	14	2
W	0	13	0	87	2
Υ	0	25	0	75	2
Z	0	7	0	93	2
AV	0	76	18	7	4
AX	0	13	0	87	4
ΑZ	0	13	87	0	4
DD.	0	83	5	12	4
BD					
BF	100	0	0	0	4



3rd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 75.61% 0.627

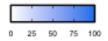
	(Interce pt)	loc.B5_ 1_SM	dip_y_ SM	fr_halo gen1	fr_halo gen2	fr_halo gen3	fr_halo gen4	fr_halo gen5	fr_halo gen6
2	0.2551	-	1.0614	-	147.49	208.18	-	-	151.14
	781	0.2626	11	1.3349	857	29	1.2895	78.966	169
		266		78			53	59	
3	309.26	-	-	-	35.509	-	-	48.874	-
	15018	86.816	80.507	204.02	02	164.64	86.822	88	59.190
		2331	978	9664		19	379		60
4	-	-	1.6357	1.6133	-	210.90	-	193.59	-
	2.1942	0.4592	47	17	40.936	59	117.84	070	24.624
	820	067			23		5590		75

1	5	1	0	1	7				
	(71%)	(14%)	(0%)	(14%)	(17%)				
2	2	12	0	2	16				
	(12%)	(75%)	(0%)	(12%)	(39%)				
3	0	0	8	0	8				
	(0%)	(0%)	(100%)	(0%)	(20%)				
4	1	3	0	6	10				
	(10%)	(30%)	(0%)	(60%)	(24%)				
total	8	16	8	9	41				
	(62%)	(75%)	(100%)	(67%)	(76%)				
,	1	2	3	4	total				
■ Accuracy ■ False ■ Precision ■ Size ■ True									

3. 3rd Place

Training Set Probability Heatmap

	1	2	3	4	Exp
Α	6	74	0	20 54 2 3 0 0 11 10 40 8 33 34 2 17 60 10 13 0 0 7 59 4 0 0 0 0 0 0 0 0 0 0 0 0 0	1
AF	24	22	0	54	1
В	60	38	0	2	1
С	49	48	0	3	1
D	88	12	0	0	1
Ε	82	18	0	0	1
F	76	13	0	11	1
AA	15	74	0	10	2
AB	1	59	0	40	2
AC	20	72	0	8	2
AH	46	21	0	33	2
AJ	0	66	0	34	2
G	51	47	0	2	2
J	8	75	0	17	2
K	0	40	0	60	2
M	19	72	0	10	2
Т	12	75	0	13	2
U	0	100	0	0	2
X	12	88	0	0	2
AL	0	100	0	0	2
AM	25	68	0	7	2
BCDEFABCHAJGJKMTUXLMHROPQRSTUNWY	60 49 88 82 76 15 1 20 46 0 51 8 0 19 12 0 25 0 42 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	22 38 48 12 18 13 74 59 72 21 66 47 75 40 72 75 100 88 100 68 41 54 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	59	11111122222222222222223333333344
R	42	54	0	4	2
AO	0	0	100	0	3
AP	0	0	100	0	3
AQ	0	0	100 100	0	3
AR	0	0	100	0	3
AS	0	0	100	0	3
ΑT	0	0	100	0	3
ΑU	0	0	100 100	0	3
AN	0	0	100 0 0	0	3
AW	0	41	0	59	4
		71	0	29	
BA	0	23	0	77	4
BB	1	9	0	90	4
BC	5	74	0	21	4
BE	1	8	0	21 92	4
BH	0	0	0	100	4
BI	51	19	0	29	4
BJ	1	8	0	91	4
BK	4	72	0	100 29 91 24	4



3. 3rd Place

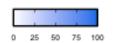
Test Set

1	0	0	0	0	0				
	(0%)	(0%)	(0%)	(0%)	(0%)				
2	2	3	6	4	15				
	(13%)	(20%)	(40%)	(27%)	(71%)				
3	0	0	0	0	0				
	(0%)	(0%)	(0%)	(0%)	(0%)				
4	1	1	3	1	6				
	(17%)	(17%)	(50%)	(17%)	(29%)				
total	3	4	9	5	21				
	(0%)	(75%)	(0%)	(20%)	(19%)				
	1	2	3	4	total				
■ Accuracy ■ False ■ Precision ■ Size ■ True									

3. 3rd Place

Test Set Probability Heatmap

	1	2	3	4	Exp
AD	0	24	0	76	2
AE	0	0	100	0	2
ΑI	9	75	0	16	2
AK	0	0	100	0	2
- 1	6	18	0	76	2
L	1	9	0	90	2
N	19	71	0	9	2
0	83	16	0	0	2
P	0	0	100	0	2
Q	0	0	100	0	2
S	0	0	100	0	2
٧	17	74	0	10	2
W	73	15	0	11	2
Υ	0	0	100	0	2
Z	1	11	0	88	2
AV	0	0	100	0	4
AX	11	20	0	69	4
ΑZ	0	0	100	0	4
BD	0	0	100	0	4
BF	91	6	0	3	4
BG	0	100	0	0	4



4th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 75.61% 0.626

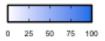
	(Interce pt)	dip_y_ P	dip_y_S M	fr_halo gen1	fr_halo gen2	fr_halo gen3	fr_halo gen4	fr_halo gen5	fr_halo gen6
2	-	0.1055	1.2410	-	207.49	361.71	-	-	226.53
	1.4680	368	38	1.3348	30199	874	1.2104	124.71	229
	27			45			86	93	
3	-	49.337	-	-	0.6740	-	15.884	195.84	-
	192.63	5233	209.21	342.94	194	99.074	257	49	72.729
	0158		9979	4812		62			45
4	-	0.1171	2.0833	1.8852	-	365.15	-	354.42	-
	5.1596	707	96	00	55.518	575	245.45	75	28.714
	75				3102		9398		10

1	4	2	0	1	7				
	(57%)	(29%)	(0%)	(14%)	(17%)				
2	1	13	0	2	16				
	(6%)	(81%)	(0%)	(12%)	(39%)				
3	0 0		8	0	8				
	(0%) (0%)		(100%)	(0%)	(20%)				
4	1	3	0	6	10				
	(10%)	(30%)	(0%)	(60%)	(24%)				
total	6	18	8	9	41				
	(67%)	(72%)	(100%)	(67%)	(76%)				
·	1	2	3	4	total				
■ Accuracy ■ False ■ Precision ■ Size ■ True									

4. 4th Place

Training Set Probability Heatmap

	1	2	3	4	Ехр
	5		0	19	
A AF	22	75	0	50	1
В	22 59	21 39	0	58 2 3 0 0 7 13 39 14 31 41	1
6		53	0	2	4
D	86	1/	0	0	4
-	88	12	0	0	4
C D E F	95	0	0	7	4
AA	85 12	14 12 8 75 60 75	0 0	12	1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3
ΔR	1	60	0	30	2
AB AC AH AJ	1 11 49	75	0	1/	5
AH	40	20	0	21	5
A I	0	50	0	//1	5
G	0 40	20 59 56	0 0 0	4	2
Ğ	17	69	0	14	2
K	0	50	0	4 14 50	5
M	0 19	73	ő	8	5
T .	24	66	ŏ	10	2
- 6	0	100	ŏ	8 10 0	2
G K M T U X	0 14 0	86	ñ	ň	2
ΑĹ	0	100	0	ň	2
AM	24	69	ŏ	0 0 7 60 3 0	2
Н	0	40	ŏ	60	5
R	46	51	ŏ	3	5
AO		0	100	ŏ	3
AP	0	ñ	100	ŏ	3
AQ	ŏ	0	100	0	3
AP AQ AR	Ö	Ö	100	Ö	3
AS	Ö	Ö	100	Ö	3
AT	Ö	0	100	0	3
AU	0	0	100	0	3
AN	0 0	0	100	Ö	3
AW	0	40	0	60	4
AY	Ö	68	Ö	32	4
ВА	Ö	24	0	76	4
ВВ	1	10	Ö	89	4
вс	4	74	Ö	89 22	4
BE	Ö	6	Ö	94	4
вн	Ö	Ö	Ö	100	4
ВІ	41	25	0	34	4
BJ	2	11	0	88	4
BK	5	74	0	21	4



4. 4th Place

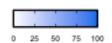
Test Set

1	0	0	0	0	0				
	(0%)	(0%)	(0%)	(0%)	(0%)				
2	2	6	1	6	15				
	(13%)	(40%)	(7%)	(40%)	(71%)				
3	0	0	0	0	0				
	(0%)	(0%)	(0%)	(0%)	(0%)				
4	1	3	1	1	6				
	(17%)	(50%)	(17%)	(17%)	(29%)				
total	3	9	2	7	21				
	(0%)	(67%)	(0%)	(14%)	(33%)				
·	1	2	3	4	total				
■ Accuracy ■ False ■ Precision ■ Size ■ True									

4. 4th Place

Test Set Probability Heatmap

	1	2	3	4	Exp
AD	0	31	0	69	2
AE	42	53	0	5	2
ΑI	9	77	0	14	2
AK	10	77	0	12	2
- 1	1	9	0	90	2
L	1	10	0	89	2
N	16	75	0	9	2
0	96	4	0	0	2
Р	0	0	100	0	2
Q	86	13	0	0	2
S	37	60	0	4	2
٧	10	76	0	14	2
W	21	17	0	62	2
Υ	27	24	0	49	2
Z	0	8	0	92	2
AV	24	70	0	7	4
AX	6	15	0	79	4
ΑZ	0	0	100	0	4
BD	10	78	0	12	4
BF	98	2	0	1	4
BG	0	100	0	0	4



5th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 78.05% 0.624

	(Inte	To tal	fr_bi cycli	fr_bi cycli	fr_bi cycli	fr_bi cycli	fr_bi cycli	fr_h alog	fr_h alog	fr_h alog	fr_h alog	fr_h alog	fr_h alog
	t)	_P	c1	c2	сЗ	с5	с6	en1	en2	en3	en4	en5	en6
2	-	1.	28.3	0	0	46.9	0	-	14.3	19.5	-	-	20.9
	6.84	06	3664			0293		2.31	269	963	9.13	27.3	305
	204	15				5		619	3	27	864	354	84
	1	52						68				5	
3	-	2.	-	0	0	-	0	-	13.0	-	-	18.8	_
	26.7	78	11.2			39.9		0.77	610	9.26	89.2	283	5.48
	876	93	8751			8767		212	5	310	418	1	265
	84	18				4		36		4	2		8
4	_	1.	27.0	0	0	-	0	_	-	20.2	_	10.9	-
	15.1	86	2322			7.23		0.13	10.4	131	98.1	084	6.62
	631	00				2256		130	168	04	133	4	931
	12	06						35	4		5		6

1	6	1	0	0	7				
	(86%)	(14%)	(0%)	(0%)	(17%)				
2	2	13	1	0	16				
	(12%)	(81%)	(6%)	(0%)	(39%)				
3	0	0	7	1	8				
	(0%)	(0%)	(88%)	(12%)	(20%)				
4	0	2	2	6	10				
	(0%)	(20%)	(20%)	(60%)	(24%)				
total	8	16	10	7	41				
	(75%)	(81%)	(70%)	(86%)	(78%)				
·	1	2	3	4	total				
■ Accuracy ■ False ■ Precision ■ Size ■ True									

5. 5th Place

Training Set Probability Heatmap

			,		-
	1	2	3	4	Exp
Α	16	74	0	10	1
AF	57	21 15	0	22 0 1 0 2 2 4 0 14 29 14 0 3 29 26 0 0 0 0 5 41 13 36 10 72 13 0 0 0 13 14 15 10 10 10 10 10 10 10 10 10 10 10 10 10	
В	85 70 96 52 93 36	15	0 0	0	1
С	70	29	0	1	1
D	96	4	0	0	1
C D E F	52	4 46	0	2	1
F	93	6 60	0	2	1
AA	36	60	0	4	2
AB	0	100	0	0	2
AB AC AH AJ	0 10 48	100 75 23 86 22 97 71 74 100 100	0 0 0 0 0 0 0	14	2
AH	48	23	0	29	2
AJ	0	86	0	14	2
G	0 78 0 0	22	0	0	2
J	0	97	0	3	2
K	0	71	0	29	2
M	0	74	0	26	2
Т	0	100	0	0	2
U	0	100	0	0	2
G K M T U X AL	0 0 4 0	96	0	0	2
AL	0	100	0	0	2
AM H	29	66 6 75	0 0 0 0 53	5	111111222222222222222333333334
н	0 12	6	53	41	2
R	12	75	0 59	13	2
AO	0	5	59	36	3
AP	0	0	90 26	10	3
AQ	0 0 0	5 0 2 1 0	26	72	3
AR	0	1	86	13	3
AS	0	0	100 100	0	3
AP AQ AR AS AT AU AN AW	0	0	100	27	3
AU	0 0 0	5	58	3/	3
AN	0	0 6	100	44	3
AVV	0	9	53	0 41 75	4
AY		25	0	75	4
BA	0	18	0	82	4
BB	1	9	1	83	4
BC	5	71	7 1 0 0	23 72 100	4
BE	0	28	0	100	4
BH	0	0	61	30	4
BI BJ	2	10	61	38 83	4
BK	6	73	1	21	4
DI	U	13		41	-



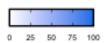
5. 5th Place

Test Set

1	0	0	0	0	0		
	(0%)	(0%)	(0%)	(0%)	(0%)		
2	1	7	3	4	15		
	(7%)	(47%)	(20%)	(27%)	(71%)		
3	0	0	0	0	0		
	(0%)	(0%)	(0%)	(0%)	(0%)		
4	0	5	0	1	6		
	(0%)	(83%)	(0%)	(17%)	(29%)		
total	1	12	3	5	21		
	(0%)	(58%)	(0%)	(20%)	(38%)		
	1	2	3	4	total		
	■ Accuracy ■ False ■ Precision ■ Size ■ True						
5. 5th Place							

Test Set Probability Heatmap

	1	2	3	4	Exp
AD	0	33	0	67	2
AE	0	2	74	24	2
ΑI	12	75	0	12	2
AK	0	94	0	6	2
- 1	24	24	1	52	2
L	0	1	0	99	2
N	1	57	4	39	2
0	0	29	0	71	2
Р	0	99	0	1	2
Q	0	96	0	4	2
S	0	96	0	4	2
٧	26	68	0	6	2
W	58	21	0	21	2
Υ	0	0	96	4	2
Z	0	0	100	0	2
AV	5	72	1	22	4
AX	7	17	2	73	4
AZ	5	73	1	21	4
BD	0	71	0	29	4
BF	0	53	0	47	4
BG	0	100	0	0	4



6th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 75.61% 0.619

	(Interce	NPA_	dip_y_	fr_halog	fr_halog	fr_halog	fr_halog	fr_halog	fr_halog
	pt)	4_P	Р	en1	en2	en3	en4	en5	en6
2	0.82332	-	0.5359	-	32.542	70.390	3.5891	-	40.820
	39	38.28	898	2.8125	78	67	39	46.784	491
		592		054				38	
3	-	331.9	10.045	-	32.770	-	-	70.324	-
	129.684	1319	9488	41.905	06	19.536	20.074	93	3.7516
	8875			0872		22	153		23
4	-	-	0.9011	-	-	72.700	-	64.706	-
	1.97052	61.02	827	0.4962	18.950	38	46.461	70	14.455
	51	157		761	69		476		536

1	5	1	0	1	7		
	(71%)	(14%)	(0%)	(14%)	(17%)		
2	2	12	0	2	16		
	(12%)	(75%)	(0%)	(12%)	(39%)		
3	0	1	7	0	8		
	(0%)	(12%)	(88%)	(0%)	(20%)		
4	0	3	0	7	10		
	(0%)	(30%)	(0%)	(70%)	(24%)		
total	7	17	7	10	41		
	(71%)	(71%)	(100%)	(70%)	(76%)		
	1	2	3	4	total		
	■ Accuracy ■ False ■ Precision ■ Size ■ True						
6	. 6th Place						

Training Set Probability Heatmap

			,		-
	1	2	3	4	Exp
Α	11	76	0	13	1
AF	15 62	20	0 0 7 0 0 0 0 0 0 0 0 0	65	1
В	62	37	0	1 0 0 1 1 3 31 8 29 11 2 34 54 18 32 0 0 0 8	111111222222222222222333333334
C D E F	93	0 0 37 4 56 67 74 19 89 49 66 46	7	0	1
D	100	0	0	0	1
E	100 62 94 40 2 18 52 0 49	37	0	1	1
F	94	4	0	1	1
AA	40	56	0	3	2
AB AC AH AJ	2	67	0	31	2
AC	18	74	0	8	2
AH	52	19	0	29	2
AJ	0	89	0	11	2
G	49	49	0	2	2
J	1 0 6	66	0	34	2
K	0	46	0	54	2
M	6	76	0	18	2
T	_1_	67	0	32	2
U	0	100	0	0	2
G J K M T U X AL	1 0 0 0 18	100	0 0 0	0	2
AL	0	100	0	0	2
AM H	18	76 67 100 100 74 29 74 0 2 0 38	0	8	2
н	0 18	29	34	36	2
R	18	74	0	36 8	2
AO	0 0 5 1	0	100	0 1 0 32 0 0 0 0 37 38	3
AP	0_	2	97	1_	3
AQ	5	0	95	0	3
AR	1	38	29	32	3
AP AQ AR AS AT AU AN	0	0	97 95 29 100 100	0	3
AT	0	0		0	3
AU	0	0	100	0	3
AN	0	0 30	100	0	3
AW	0 0 0 0	30	33	37	4
AY		62	0	38	4
BA	0	2 18	0	98	4
ВВ	15	18	0	66	4
вс	3	73	0	24	4
BE	13	19	0	69	4
ВН	0	0		100	4
BI	4	11	5	79 91	4
BJ	1	8	0	91	4
BK	14	76	0	10	4



6. 6th Place

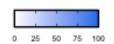
Test Set

1	0	0	0	0	0
	(0%)	(0%)	(0%)	(0%)	(0%)
2	2	7	1	5	15
	(13%)	(47%)	(7%)	(33%)	(71%)
3	0	0	0	0	0
	(0%)	(0%)	(0%)	(0%)	(0%)
4	2	4	0	0	6
	(33%)	(67%)	(0%)	(0%)	(29%)
total	4 (0%)	11 (64%)	1 (0%)	5 (0%)	21 (33%)
total	4	11	1 (0%)		

6. 6th Place

Test Set Probability Heatmap

	1	2	3	4	Exp
AD	0	80	0	20	2
AE	0	29	0	71	2
ΑI	2	68	0	30	2
AK	3	71	0	27	2
-1	35	20	0	45	2
L	1	7	0	93	2
N	2	70	0	28	2
0	60	39	0	1	2
Р	12	76	0	11	2
Q	0	43	0	57	2
S	7	76	0	17	2
٧	9	77	0	14	2
W	100	0	0	0	2
Υ	10	16	0	74	2
Z	0	0	100	0	2
AV	1	65	0	34	4
AX	48	20	0	32	4
AZ	11	76	0	13	4
BD	1	61	0	38	4
BF	100	0	0	0	4
BG	0	100	0	0	4



7th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

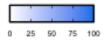
accuracy_formatted McFadden_R2 68.29% 0.61

	(Intercept)	L_1_SM	dip_y_SM	fr_aryl_methyl1	fr_aryl_methyl2
2	-2.835825	0.313488	0.8895763	2.117777	-16.77958
3	67.818608	-11.106972	-5.7627283	-14.193321	-15.81635
4	15.709301	-2.297570	-0.2509154	-14.906936	-24.89733

1	2	3	0	2	7
	(29%)	(43%)	(0%)	(29%)	(17%)
2	1	12	0	3	16
	(6%)	(75%)	(0%)	(19%)	(39%)
3	0	0	7	1	8
	(0%)	(0%)	(88%)	(12%)	(20%)
4	1	1	1	7	10
	(10%)	(10%)	(10%)	(70%)	(24%)
total	4	16	8	13	41
	(50%)	(75%)	(88%)	(54%)	(68%)
·	1	2	3	4	total
	■ Accura	cy I Fals	e 🔲 Precis	sion 🗖 Siz	e 🔳 True
7	. 7th Place				

Training Set Probability Heatmap

A 100 0 0 0 1 AF 9 91 0 0 1 B 27 19 0 54 1 C 27 30 0 42 1 D 38 61 0 0 1 E 100 0 0 0 1 F 44 56 0 0 1 AA 19 70 0 11 2 AB 7 84 0 9 2 AC 14 85 0 0 2 AJ 58 40 0 3 2 G 23 77 0 0 2 J 3 97 0 0 2 AJ 58 40 0 3 2 G 23 77 0 0 2 J 3 97 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 2 AM 7 93 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 3 AM 7 93 0 0 2 AM 7 93 0 0 2 AM 7 93 0 0 3 AM 7 93 0 0 3 AN 0 0 93 7 3 AP 0 0 80 19 AQ 0 0 97 3 3 AR 3 1 75 21 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AW 2 39 0 59 4 AY 36 12 1 52 4 BA 0 0 71 29 4 BB 2 8 0 89 BC 2 7 0 91 4 BB 7 82 0 11 BH 42 18 0 39 BI 3 2 47 49 BB B 2 8 0 89 BC 7 82 0 11 BH 42 18 0 39 BI 3 2 47 49 BB B 2 8 0 89 BB 2 8 0 89 BB 3 2 47 49 BB B 3 2 47 49 BB B 3 2 47 49 BB B 3 3 2 47 49 BB A 3 4 48		1	2	3	4	Ехр
AF 9 91 0 0 1 B 27 19 0 54 1 C 27 30 0 42 1 D 38 61 0 0 1 E 100 0 0 0 1 F 44 56 0 0 1 AA 19 70 0 11 AB 7 84 0 9 AC 14 85 0 0 2 AJ 58 40 0 3 G 23 77 0 0 2 AJ 58 40 0 3 G 23 77 0 0 2 K 23 77 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 2 AM 7 93 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 2 AM 7 93 0 0 3 AR 3 1 75 21 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AU 1 1 36 62 3 AN 0 0 100 0 3 AW 2 39 0 59 4 AY 36 12 1 52 4	Α	100	0	0	0	1
C 27 30 0 42 1 D 38 61 0 0 1 E 100 0 0 0 1 F 44 56 0 0 1 AA 19 70 0 11 2 AB 7 84 0 9 AC 14 85 0 0 2 AH 15 85 0 0 2 AJ 58 40 0 3 2 G 23 77 0 0 2 K 23 77 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 2 AM 7 93 0 0 2 AN 7 93 0 0 2 AN 7 93 0 0 3 AT 0 0 80 19 AQ 0 0 97 3 AR 3 1 75 21 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AU 1 1 36 62 AN 0 0 100 0 3 AW 2 39 0 59 4 AY 36 12 1 52	AF	9	91	0	0	1
C 27 30 0 42 1 D 38 61 0 0 1 E 100 0 0 0 1 F 44 56 0 0 1 AA 19 70 0 11 2 AB 7 84 0 9 AC 14 85 0 0 2 AH 15 85 0 0 2 AJ 58 40 0 3 2 G 23 77 0 0 2 K 23 77 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 2 X 10 90 0 1 2 AL 8 92 0 0 2 AM 7 93 0 0 2 AN 7 93 0 0 2 AN 7 93 0 0 3 AT 0 0 80 19 AQ 0 0 97 3 AR 3 1 75 21 3 AS 0 0 100 0 3 AT 0 0 100 0 3 AU 1 1 36 62 AN 0 0 100 0 3 AW 2 39 0 59 4 AY 36 12 1 52	В	27	19	0	54	1
AY 36 12 1 52 4	С	27	30	0	42	1
AY 36 12 1 52 4	D	38	61	0	0	1
AY 36 12 1 52 4	Ε	100	0	0	0	1
AY 36 12 1 52 4	F	44	56	0	0	1
AY 36 12 1 52 4	AA	19	70	0	11	2
AY 36 12 1 52 4	AB	7	84	0	9	2
AY 36 12 1 52 4	AC	14	85	0	0	2
AY 36 12 1 52 4	AH	15	85	0	0	2
AY 36 12 1 52 4	AJ	58	40	0	3	2
AY 36 12 1 52 4	G	23	77	0	0	2
AY 36 12 1 52 4	J	3	97	0	0	2
AY 36 12 1 52 4	K	23	77	0	0	2
AY 36 12 1 52 4	M	15	28	0	57	2
AY 36 12 1 52 4	T	13	37	0	50	2
AY 36 12 1 52 4	U	22	78	0	0	2
AY 36 12 1 52 4	Х	10	90	0	1_	2
AY 36 12 1 52 4	AL	8	92	0	0	2
AY 36 12 1 52 4	AM	7	93	0	0	2
AY 36 12 1 52 4		2	39	0	59	2
AY 36 12 1 52 4	R	13	87	0	0	2
AY 36 12 1 52 4	AO	0	0	93	7	3
AY 36 12 1 52 4	AP	0	0	80	19	3
AY 36 12 1 52 4	AQ	0	0	97	3	3
AY 36 12 1 52 4	AR	3	1	75	21	3
AY 36 12 1 52 4	AS	0	0	100	0	3
AY 36 12 1 52 4	AT	0	0	100	0	3
AY 36 12 1 52 4	AU	1	1	36	62	3
AY 36 12 1 52 4	AN	0	0		0	3
BA 0 0 71 29 4 BB 2 8 0 89 4 BC 2 7 0 91 4 BE 7 82 0 11 4 BH 42 18 0 39 4 BI 3 2 47 49 4 BJ 2 8 0 89 4 BK 2 6 0 92 4	AW	2				
BA 0 0 71 29 4 BB 2 8 0 89 4 BC 2 7 0 91 4 BE 7 82 0 11 4 BH 42 18 0 39 4 BI 3 2 47 49 4 BJ 2 8 0 89 4 BK 2 6 0 92 4		36	12	1	52	4
BB 2 8 0 89 4 BC 2 7 0 91 4 BE 7 82 0 11 4 BH 42 18 0 39 4 BI 3 2 47 49 4 BJ 2 8 0 89 4 BK 2 6 0 92 4		0	0	/1	29	4
BE 7 82 0 11 4 BH 42 18 0 39 4 BI 3 2 47 49 4 BJ 2 8 0 89 4 BK 2 6 0 92 4		2	8	0	89	4
BH 42 18 0 39 4 BI 3 2 47 49 4 BJ 2 8 0 89 4 BK 2 6 0 92 4		2	/	0	91	4
BI 3 2 47 49 4 BJ 2 8 0 89 4 BK 2 6 0 92 4	BE	40	82	0	77	4
BJ 2 8 0 89 4 BK 2 6 0 92 4		42	18	47	40	4
BK 2 6 0 92 4	RI	3	2	47	49	4
DR 2 0 0 92 4		2		0		4
	ΒK		0	U	92	4



7. 7th Place

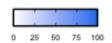
Test Set

1	0	0	0	0	0	
	(0%)	(0%)	(0%)	(0%)	(0%)	
2	1	7	3	4	15	
	(7%)	(47%)	(20%)	(27%)	(71%)	
3	0	0	0	0	0	
	(0%)	(0%)	(0%)	(0%)	(0%)	
4	0	2	2	2	6	
	(0%)	(33%)	(33%)	(33%)	(29%)	
total	1	9	5	6	21	
	(0%)	(78%)	(0%)	(33%)	(43%)	
	1	2	3	4	total	
■ Accuracy ■ False ■ Precision ■ Size ■ True						

7. 7th Place

Test Set Probability Heatmap

	1	2	3	4	Exp
AD	23	77	0	0	2
AE	1	1	43	55	2
AI	2	4	3	92	2
AK	7	93	0	0	2
-1	10	79	0	10	2
L	2	8	0	90	2
N	1	1	40	58	2
0	64	22	0	14	2
Р	0	0	100	0	2
Q	0	0	100	0	2
S	0	0	98	2	2
٧	17	60	0	22	2
W	1	99	0	0	2
Υ	7	93	0	0	2
Z	3	97	0	0	2
AV	2	2	33	63	4
AX	3	97	0	0	4
ΑZ	0	0	100	0	4
BD	2	3	9	87	4
BF	9	2	47	41	4
BG	16	78	0	5	4



8th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 78.05% 0.608

Model Coefficients

	(Interc	Total_	fr_ester	fr_es	fr_hal	fr_hal	fr_hal	fr_halo	fr_hal	fr_hal
	ept)	Р	1	ter2	ogen1	ogen2	ogen3	gen4	ogen5	ogen6
2	-	0.660	1.25057	-	-	348.9	544.4	-	-	239.0
	3.7454	0579	94	308.	3.221	224	9708	6.1909	504.7	28505
	85			3376	9940			58	868	
3	-	173.9	-	636.	360.4	585.5	-	-	131.3	5.884
	2235.4	46284	1974.62	4967	65362	380	99.57	1970.2	856	706
	98567	4	22393		8		157	88392		
4	-	0.880	-	-	0.080	-	545.6	-	613.0	-
	7.0129	3573	0.53673	202.	7997	361.6	4455	1460.1	888	127.9
	22		52	3241		937		96495		12964

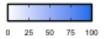
Training Set

1	5	2	0	0	7			
	(71%)	(29%)	(0%)	(0%)	(17%)			
2	2	12	0	2	16			
	(12%)	(75%)	(0%)	(12%)	(39%)			
3	0	0	8	0	8			
	(0%)	(0%)	(100%)	(0%)	(20%)			
4	0	3	0	7	10			
	(0%)	(30%)	(0%)	(70%)	(24%)			
total	7	17	8	9	41			
	(71%)	(71%)	(100%)	(78%)	(78%)			
·	1	2	3	4	total			
■ Accuracy ■ False ■ Precision ■ Size ■ True								

8.8th Place

Training Set
Probability Heatmap

	1	2	3	4	Exp	
Α	16	69	0	15	1	
AF	50	8	0	43	1	
В	62	35	0	4	1111122222222222222333333334	
C D E	48	46 11 55 14 87 45 71 8 62 41 67 56 69	0	4 6 0	1	
D	89	11	0	0	1	
E	36	55	0	8	1	
F	78 11 0 12	14	0 0 0 0 0 0 0	9	1	
AA	11	87	0	3	2	
AB	0	45	0	55	2	
AC AH AJ	12	71	0	17	2	
AH	44	8	0	48	2	
AJ	0	62	0	38	2	
G	54	41	0	5	2	
J	20	67	0	13	2	
K	0	56	0	44	2	
M	44 0 54 20 0 2 83	69	0	28	2	
T	83	15 100	0	1	2	
U	0	100	0	0	2	
G K M T U X AL	11	89	0	0	2	
AL	0 11 0	100	0 0	0	2	
AM	24	100 64 61 70	0	9 3 55 17 48 38 5 13 44 28 1 0 0 0 12 39 16 0	2	
Н	_1_	61	Ö	39	2	
R	13	70	0	16	2	
AO	0 0 0	0 0 0	100	0	3	
AP	0	0	100	0	3	
AQ	0	0	100	0 0 0	3	
AR	0	0	100	0	3	
AS	0	0	100	0	3	
AP AQ AR AS AT AU AN AW	0	0	100	0	3	
AU	0 0 1 0	0	100	0 0 39 58	3	
AN	0	0 61	100	0	3	
	1_	61	0	39	4	
AY		42		58	4	
BA	0	39	0	61	4	
ВВ	8	8	0	83	4	
вс	8	72	0	20	4	
BE	8	8	0	84	4	
ВН		0	0	100	4	
BI	1	22	0	77	4	
BJ	11	33	0	56	4	
BK	9	72	0	19	4	



8. 8th Place

Test Set

1	0	0	0	0	0			
	(0%)	(0%)	(0%)	(0%)	(0%)			
2	1	7	5	2	15			
	(7%)	(47%)	(33%)	(13%)	(71%)			
3	0	0	0	0	0			
	(0%)	(0%)	(0%)	(0%)	(0%)			
4	0	3	1	2	6			
	(0%)	(50%)	(17%)	(33%)	(29%)			
total	1	10	6	4	21			
	(0%)	(70%)	(0%)	(50%)	(43%)			
·	1	2	3	4	total			
■ Accuracy ■ False ■ Precision ■ Size ■ True								

8. 8th Place

Error in if (as.numeric(verif\$Exp[i]) == where.is.sec) {: the condition has length > 1

9th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 75.61% 0.607

Model Coefficients

	(Interce	NPA_7	dip_y_	fr_halog	fr_halog	fr_halog	fr_halog	fr_halog	fr_halog
	pt)	_SM	SM	en1	en2	en3	en4	en5	en6
2	-	-	1.6920	-	141.02	216.42	-	-	177.40
	3.6727	20.428	58	0.8991	034	89	3.3598	122.27	557
	34	60		306			81	12	
3	-	_	-	-	93.731	-	-	167.02	-
	98.733	639.59	23.491	29.038	48	126.94	165.71	90	68.536
	056	659	699	6674		16	5348		95
4	-	_	2.7137	2.8480	-	220.34	-	204.14	-
	7.9045	20.888	80	305	42.161	61	146.95	28	23.225
	53	27			24		9118		76

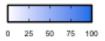
Training Set

1	4	2	0	1	7			
	(57%)	(29%)	(0%)	(14%)	(17%)			
2	0	13	0	3	16			
	(0%)	(81%)	(0%)	(19%)	(39%)			
3	0	0	8	0	8			
	(0%)	(0%)	(100%)	(0%)	(20%)			
4	0	3	1	6	10			
	(0%)	(30%)	(10%)	(60%)	(24%)			
total	4	18	9	10	41			
	(100%)	(72%)	(89%)	(60%)	(76%)			
,	1	2	3	4	total			
■ Accuracy ■ False ■ Precision ■ Size ■ True								

9. 9th Place

Training Set
Probability Heatmap

	1	2	3	4	Exp
Α	10	74	0	17 54 1 3 0 0 7 14 41 15 45 41 3 16 51 6 9 0 0 0 5 64 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1
AF	30	15	0	54	1
В	77	23	0	1	1
С	35	63	0	3	1
D	96	4	0	0	1
Ε	93	7	0	0	1
F	84	8	0	7	1
AA	1	86	0	14	2
AB	0	58	0	41	2
AC	2	83	0	15	2
AH	30	25	0	45	2
AJ	0	59	0	41	2
G	43	54	0	3	2
J	5	79	0	16	2
K	0	49	0	51	2
M	21	72	0	6	2
Т	31	60	0	9	2
U	0	100	0	0	2
Х	4	96	0	0	2
AL	0	100	0	0	2
AFBCDEFABCHAJGJKMTUXLMHROPQRSTUNWY	30 77 35 96 93 84 1 0 2 30 0 43 5 0 21 31 0 4 0 28 0 0 48 0 0 0 0 0 0 0 0 0 0 0 0 0	15 23 63 4 7 8 86 58 83 25 59 54 79 49 72 60 100 96 100 67 36 50 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	5	11111122222222222222223333333344
Н	0	36	0	64	2
R	48	50	0	2	2
AO	0	0	100	0	3
AP	0	0	100	0	3
AQ	0	0	100	0	3
AR	0	0	100 100 100	0	3
AS	0	0	100	0	3
AT	17	25	34	24	3
AU	0	0	100 72 0	0	3
AN	0	0	72	28	3
AW	0	36	0	64	4
	0	66	0	34	
BA	0	25	0	75	4
ВВ	0	6	0	94	4
ВС	6	74	0	20	4
BE	0	3	0	97	4
ВН	0	0	28	20 97 72 18	4
ВІ	3	13	66	18	4
BJ	36	5	0	59	4
BK	0	78	0	22	4



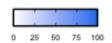
9. 9th Place

Test Set

1	0	0	0	0	0			
	(0%)	(0%)	(0%)	(0%)	(0%)			
2	5	3	2	5	15			
	(33%)	(20%)	(13%)	(33%)	(71%)			
3	0	0	0	0	0			
	(0%)	(0%)	(0%)	(0%)	(0%)			
4	3	1	1	1	6			
	(50%)	(17%)	(17%)	(17%)	(29%)			
total	8	4	3	6	21			
	(0%)	(75%)	(0%)	(17%)	(19%)			
·	1	2	3	4	total			
	■ Accuracy ■ False ■ Precision ■ Size ■ True							
9	. 9th Place							

Test Set Probability Heatmap

	1	2	3	4	Exp
AD	0	23	0	77	2
AE	96	4	0	0	2
AI	99	1	0	0	2
AK	20	71	0	9	2
- 1	0	5	0	95	2
L	0	7	0	93	2
N	79	19	0	2	2
0	0	0	100	0	2
P	100	0	0	0	2
Q	100	0	0	0	2
S	24	73	0	3	2
٧	9	78	0	12	2
W	0	14	0	85	2
Υ	0	7	75	17	2
Z	1	6	0	93	2
AV	100	0	0	0	4
AX	1	11	0	88	4
ΑZ	0	0	100	0	4
BD	99	1	0	0	4
BF	87	10	0	4	4
BG	0	100	0	0	4



10th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted McFadden_R2 75.61% 0.605

Model Coefficients

	(Interce		para_	fr_halo	fr_halo	fr_halo	fr_halog	fr_halo	fr_halo
	pt)	dip_y_P	Р	gen1	gen2	gen3	en4	gen5	gen6
2	-	0.2799	0.034	-	240.03	425.87	-	-	254.05
	56.3813	346	6653	1.4888	66	53	0.22606	228.52	247
	7			94			06	15	
3	-	107.14	7.965	-	242.49	-	-	383.13	-
	14112.7	73058	0291	50.202	01	150.38	235.162	58	32.400
	2044			532		79	0139		06
4	-	0.5434	0.094	1.2729	-	427.16	-	363.11	-
	156.325	941	4583	80	112.25	00	298.464	59	81.813
	49				15		9422		97

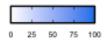
Training Set

1	4	2	0	1	7			
	(57%)	(29%)	(0%)	(14%)	(17%)			
2	1	13	0	2	16			
	(6%)	(81%)	(0%)	(12%)	(39%)			
3	0	0	8	0	8			
	(0%)	(0%)	(100%)	(0%)	(20%)			
4	0	4	0	6	10			
	(0%)	(40%)	(0%)	(60%)	(24%)			
total	5	19	8	9	41			
	(80%)	(68%)	(100%)	(67%)	(76%)			
	1	2	3	4	total			
■ Accuracy ■ False ■ Precision ■ Size ■ True								

10. 10th Place

Training Set
Probability Heatmap

	1	2	3	4	Exp
Α	3	40	0	57 27 4 1 0 6 1 17 14 2 38 22 9 5 51 11 41 0 0 0 8 41 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1
AF	48	25	0	27	1
В	34	62	0	4	1
С	53	46	0	1	1
AF BCDEFAAABACAHAJ	76	24	0	0	1
Ε	36	57	0	6	1
F	92	7	0	1	1
AA	17	66	0	17	2
AB	13	73	0	14	2
AC	41	57	0	2	2
AΗ	38	24	0	38	2
AJ	0	78	0	22	2
G	28	62	0	9	2
J	48	47	0	5	2
K	0	49	0	51	2
M	19	70	0	11	2
Т	14	45	0	41	2
U	0	100	0	0	2
Х	24	76	0	0	2
AL	0	100	0	0	2
G J K M T U X AL AM H	24	68	0	8	2
Н	3	56	0	41	2
R AO AP AQ AR AS AT AU AN AW	34 53 76 36 92 17 13 41 38 0 28 48 0 19 14 0 24 0 24 3 39 0 0 0 0 0 0 0 0 0 0 0	25 62 46 24 57 7 66 73 57 24 78 62 47 49 70 45 100 76 100 68 56 58 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	2	11111122222222222222223333333344
AO	0	0	100	0	3
AP	0	0	100	0	3
AQ	0	0	97 100	3	3
AR	0	0	100	0	3
AS	0	0	100	0	3
AT	0	0	100 100	0	3
AU	0	0	100	0	3
AN	0	0	100 0 0	0	3
AW	3	56	0	41	4
AY		66	0	34	
BA	0	6	0	94	4
ВВ	0	2	3	94	4
ВС	11	69	0	20 99	4
BE	0	1	1	99	4
ВН	0	0	0	100	4
ВІ	8	19	0	73	4
BJ	15	21	0	64	4
BK	14	68	0	18	4



10. 10th Place

Test Set

1	0	0	0	0	0		
	(0%)	(0%)	(0%)	(0%)	(0%)		
2	6	6	2	1	15		
	(40%)	(40%)	(13%)	(7%)	(71%)		
3	0	0	0	0	0		
	(0%)	(0%)	(0%)	(0%)	(0%)		
4	1	3	1	1	6		
	(17%)	(50%)	(17%)	(17%)	(29%)		
total	7	9	3	2	21		
	(0%)	(67%)	(0%)	(50%)	(33%)		
·	1	2	3	4	total		
■ Accuracy ■ False ■ Precision ■ Size ■ True							

10. 10th Place

Test Set Probability Heatmap

	1	2	3	4	Exp
AD	0	95	0	5	2
AE	59	39	0	3	2
Al	6	58	0	35	2
AK	8	65	0	28	2
- 1	38	28	0	34	2
L	0	1	85	14	2
N	25	69	0	5	2
0	86	13	0	0	2
Р	8	60	0	32	2
Q	73	27	0	1	2
S	57	43	0	0	2
V	23	69	0	8	2
W	84	11	0	5	2
Υ	7	15	0	78	2
Z	0	0	100	0	2
AV	11	67	0	22	4
AX	10	14	0	76	4
AZ	6	60	0	35	4
BD	0	0	100	0	4
BF	90	7	0	4	4
BG	0	100	0	0	4

