

# 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 ~ loc.B5_1_SM + dip_y_SM + fr_halogen	0.627
class ~ dip_y_P + dip_y_SM + fr_halogen	0.626
class ~ Total_P + fr_bicyclic + fr_halogen	0.624
class ~ NPA_4_P + dip_y_P + fr_halogen	0.619
class ~ 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

Model Coefficients

	(Interce pt)	L_1_SM	dip_y_ SM	fr_halo gen1	fr_halo gen2	fr_halo gen3	fr_halo gen4	fr_halo gen5	fr_halo gen6
2	-	0.41068	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

## Training Set

1	4 (57%)	2 (29%)	0 (0%)	1 (14%)	7 (17%)
2	2 (12%)	12 (75%)	0 (0%)	2 (12%)	16 (39%)
3	0 (0%)	0 (0%)	8 (100%)	0 (0%)	8 (20%)
4	1 (10%)	3 (30%)	0 (0%)	6 (60%)	10 (24%)
total	7 (57%)	17 (71%)	8 (100%)	9 (67%)	41 (73%)
	1	2	3	4	total

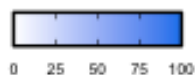
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

1. 1st Place

# Training Set

## Probability Heatmap

	1	2	3	4	Exp
A	9	56	0	35	1
AF	18	12	0	70	1
B	68	31	0	1	1
C	48	50	0	3	1
D	82	18	0	0	1
E	86	14	0	0	1
F	69	30	0	2	1
AA	11	83	0	6	2
AB	1	81	0	18	2
AC	6	92	0	2	2
AH	46	11	0	44	2
AJ	0	89	0	11	2
G	17	83	0	0	2
J	10	74	0	16	2
K	0	32	0	68	2
M	26	67	0	8	2
T	14	74	0	11	2
U	0	100	0	0	2
X	18	82	0	0	2
AL	0	100	0	0	2
AM	30	64	0	6	2
H	0	40	0	60	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
AU	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
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
BK	8	56	0	36	4



1. 1st Place

## Test Set

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

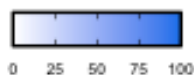
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

1. 1st Place

## Test Set

### Probability Heatmap

	1	2	3	4	Exp
AD	0	90	0	10	2
AE	0	0	100	0	2
AI	15	56	0	29	2
AK	21	55	0	25	2
I	3	30	0	68	2
L	2	8	0	90	2
N	0	0	100	0	2
O	88	12	0	0	2
P	0	0	100	0	2
Q	0	0	100	0	2
S	0	0	100	0	2
V	11	81	0	8	2
W	3	96	0	0	2
Y	45	34	0	21	2
Z	1	7	0	91	2
AV	0	0	100	0	4
AX	8	27	0	64	4
AZ	0	0	100	0	4
BD	21	54	0	25	4
BF	94	4	0	2	4
BG	0	100	0	0	4



1. 1st Place

## 2nd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
80.49%	0.645

Model Coefficients

	(Interce pt)	NPA_ 1_P	dip_y _SM	fr_halog en1	fr_halog en2	fr_halog en3	fr_halog en4	fr_halog en5	fr_halog 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

## Training Set

1	7 (100%)	0 (0%)	0 (0%)	0 (0%)	7 (17%)
2	0 (0%)	13 (81%)	2 (12%)	1 (6%)	16 (39%)
3	0 (0%)	2 (25%)	6 (75%)	0 (0%)	8 (20%)
4	0 (0%)	3 (30%)	0 (0%)	7 (70%)	10 (24%)
total	7 (100%)	18 (72%)	8 (75%)	8 (88%)	41 (80%)
	1	2	3	4	total

■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

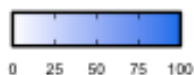
2. 2nd Place



# Training Set

## Probability Heatmap

	1	2	3	4	Exp
A	100	0	0	0	1
AF	94	1	1	4	1
B	100	0	0	0	1
C	100	0	0	0	1
D	100	0	0	0	1
E	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
T	2	66	24	9	2
U	0	100	0	0	2
X	0	100	0	0	2
AL	0	83	17	0	2
AM	0	64	30	6	2
H	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
AT	0	12	76	12	3
AU	0	76	15	8	3
AN	0	0	61	39	3
AW	0	38	0	62	4
AY	0	69	0	31	4
BA	0	25	0	75	4
BB	0	7	0	93	4
BC	0	77	2	21	4
BE	0	4	0	96	4
BH	0	0	39	61	4
BI	0	34	2	64	4
BJ	0	9	0	91	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 (17%)	3 (50%)	1 (17%)	1 (17%)	6 (29%)
total	4 (0%)	8 (62%)	2 (0%)	7 (14%)	21 (29%)
	1	2	3	4	total

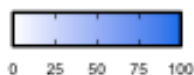
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

2. 2nd Place

## Test Set

### Probability Heatmap

	1	2	3	4	Exp
AD	0	28	0	72	2
AE	0	49	46	4	2
AI	0	82	2	16	2
AK	0	79	10	11	2
I	0	7	0	93	2
L	0	8	0	92	2
N	0	54	41	5	2
O	100	0	0	0	2
P	0	2	98	0	2
Q	100	0	0	0	2
S	100	0	0	0	2
V	0	81	5	14	2
W	0	13	0	87	2
Y	0	25	0	75	2
Z	0	7	0	93	2
AV	0	76	18	7	4
AX	0	13	0	87	4
AZ	0	13	87	0	4
BD	0	83	5	12	4
BF	100	0	0	0	4
BG	0	100	0	0	4



2. 2nd Place

### 3rd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
75.61%	0.627

Model Coefficients

	(Intercept)	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

## Training Set

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

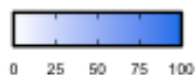
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

3. 3rd Place

# Training Set

## Probability Heatmap

	1	2	3	4	Exp
A	6	74	0	20	1
AF	24	22	0	54	1
B	60	38	0	2	1
C	49	48	0	3	1
D	88	12	0	0	1
E	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
T	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
H	0	41	0	59	2
R	42	54	0	4	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
AU	0	0	100	0	3
AN	0	0	100	0	3
AW	0	41	0	59	4
AY	0	71	0	29	4
BA	0	23	0	77	4
BB	1	9	0	90	4
BC	5	74	0	21	4
BE	1	8	0	92	4
BH	0	0	0	100	4
BI	51	19	0	29	4
BJ	1	8	0	91	4
BK	4	72	0	24	4



3. 3rd Place

## Test Set

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

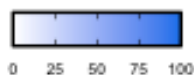
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

3. 3rd Place

## Test Set

### Probability Heatmap

	1	2	3	4	Exp
AD	0	24	0	76	2
AE	0	0	100	0	2
AI	9	75	0	16	2
AK	0	0	100	0	2
I	6	18	0	76	2
L	1	9	0	90	2
N	19	71	0	9	2
O	83	16	0	0	2
P	0	0	100	0	2
Q	0	0	100	0	2
S	0	0	100	0	2
V	17	74	0	10	2
W	73	15	0	11	2
Y	0	0	100	0	2
Z	1	11	0	88	2
AV	0	0	100	0	4
AX	11	20	0	69	4
AZ	0	0	100	0	4
BD	0	0	100	0	4
BF	91	6	0	3	4
BG	0	100	0	0	4



3. 3rd Place



## 4th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
75.61%	0.626

Model Coefficients

	(Intercept)	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

## Training Set

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

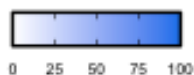
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

4. 4th Place

# Training Set

## Probability Heatmap

	1	2	3	4	Exp
A	5	75	0	19	1
AF	22	21	0	58	1
B	59	39	0	2	1
C	44	53	0	3	1
D	86	14	0	0	1
E	88	12	0	0	1
F	85	8	0	7	1
AA	12	75	0	13	2
AB	1	60	0	39	2
AC	11	75	0	14	2
AH	49	20	0	31	2
AJ	0	59	0	41	2
G	40	56	0	4	2
J	17	69	0	14	2
K	0	50	0	50	2
M	19	73	0	8	2
T	24	66	0	10	2
U	0	100	0	0	2
X	14	86	0	0	2
AL	0	100	0	0	2
AM	24	69	0	7	2
H	0	40	0	60	2
R	46	51	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
AU	0	0	100	0	3
AN	0	0	100	0	3
AW	0	40	0	60	4
AY	0	68	0	32	4
BA	0	24	0	76	4
BB	1	10	0	89	4
BC	4	74	0	22	4
BE	0	6	0	94	4
BH	0	0	0	100	4
BI	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 (13%)	6 (40%)	1 (7%)	6 (40%)	15 (71%)
3	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
4	1 (17%)	3 (50%)	1 (17%)	1 (17%)	6 (29%)
total	3 (0%)	9 (67%)	2 (0%)	7 (14%)	21 (33%)
	1	2	3	4	total

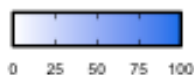
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

4. 4th Place

## Test Set

### Probability Heatmap

	1	2	3	4	Exp
AD	0	31	0	69	2
AE	42	53	0	5	2
AI	9	77	0	14	2
AK	10	77	0	12	2
I	1	9	0	90	2
L	1	10	0	89	2
N	16	75	0	9	2
O	96	4	0	0	2
P	0	0	100	0	2
Q	86	13	0	0	2
S	37	60	0	4	2
V	10	76	0	14	2
W	21	17	0	62	2
Y	27	24	0	49	2
Z	0	8	0	92	2
AV	24	70	0	7	4
AX	6	15	0	79	4
AZ	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

Model Coefficients

	(Inte rcep t)	To tal _P	fr_bi cycli c1	fr_bi cycli c2	fr_bi cycli c3	fr_bi cycli c5	fr_bi cycli c6	fr_h alog en1	fr_h alog en2	fr_h alog en3	fr_h alog en4	fr_h alog en5	fr_h alog 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

## Training Set

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

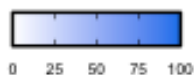
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

5. 5th Place

# Training Set

## Probability Heatmap

	1	2	3	4	Exp
A	16	74	0	10	1
AF	57	21	0	22	1
B	85	15	0	0	1
C	70	29	0	1	1
D	96	4	0	0	1
E	52	46	0	2	1
F	93	6	0	2	1
AA	36	60	0	4	2
AB	0	100	0	0	2
AC	10	75	0	14	2
AH	48	23	0	29	2
AJ	0	86	0	14	2
G	78	22	0	0	2
J	0	97	0	3	2
K	0	71	0	29	2
M	0	74	0	26	2
T	0	100	0	0	2
U	0	100	0	0	2
X	4	96	0	0	2
AL	0	100	0	0	2
AM	29	66	0	5	2
H	0	6	53	41	2
R	12	75	0	13	2
AO	0	5	59	36	3
AP	0	0	90	10	3
AQ	0	2	26	72	3
AR	0	1	86	13	3
AS	0	0	100	0	3
AT	0	0	100	0	3
AU	0	5	58	37	3
AN	0	0	100	0	3
AW	0	6	53	41	4
AY	0	25	0	75	4
BA	0	18	0	82	4
BB	1	9	7	83	4
BC	5	71	1	23	4
BE	0	28	0	72	4
BH	0	0	0	100	4
BI	0	0	61	38	4
BJ	2	10	6	83	4
BK	6	73	1	21	4



5. 5th Place



## Test Set

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	1 (7%)	7 (47%)	3 (20%)	4 (27%)	15 (71%)
3	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
4	0 (0%)	5 (83%)	0 (0%)	1 (17%)	6 (29%)
total	1 (0%)	12 (58%)	3 (0%)	5 (20%)	21 (38%)
	1	2	3	4	total

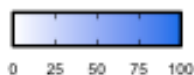
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

5. 5th Place

## Test Set

### Probability Heatmap

	1	2	3	4	Exp
AD	0	33	0	67	2
AE	0	2	74	24	2
AI	12	75	0	12	2
AK	0	94	0	6	2
I	24	24	1	52	2
L	0	1	0	99	2
N	1	57	4	39	2
O	0	29	0	71	2
P	0	99	0	1	2
Q	0	96	0	4	2
S	0	96	0	4	2
V	26	68	0	6	2
W	58	21	0	21	2
Y	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



5. 5th Place

## 6th Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

accuracy_formatted	McFadden_R2
75.61%	0.619

Model Coefficients

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

## Training Set

1	5 (71%)	1 (14%)	0 (0%)	1 (14%)	7 (17%)
2	2 (12%)	12 (75%)	0 (0%)	2 (12%)	16 (39%)
3	0 (0%)	1 (12%)	7 (88%)	0 (0%)	8 (20%)
4	0 (0%)	3 (30%)	0 (0%)	7 (70%)	10 (24%)
total	7 (71%)	17 (71%)	7 (100%)	10 (70%)	41 (76%)
	1	2	3	4	total

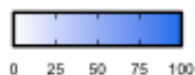
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

6. 6th Place

# Training Set

## Probability Heatmap

	1	2	3	4	Exp
A	11	76	0	13	1
AF	15	20	0	65	1
B	62	37	0	1	1
C	93	0	7	0	1
D	100	0	0	0	1
E	62	37	0	1	1
F	94	4	0	1	1
AA	40	56	0	3	2
AB	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	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
X	0	100	0	0	2
AL	0	100	0	0	2
AM	18	74	0	8	2
H	0	29	34	36	2
R	18	74	0	8	2
AO	0	0	100	0	3
AP	0	2	97	1	3
AQ	5	0	95	0	3
AR	1	38	29	32	3
AS	0	0	100	0	3
AT	0	0	100	0	3
AU	0	0	100	0	3
AN	0	0	100	0	3
AW	0	30	33	37	4
AY	0	62	0	38	4
BA	0	2	0	98	4
BB	15	18	0	66	4
BC	3	73	0	24	4
BE	13	19	0	69	4
BH	0	0	0	100	4
BI	4	11	5	79	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 (13%)	7 (47%)	1 (7%)	5 (33%)	15 (71%)
3	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
4	2 (33%)	4 (67%)	0 (0%)	0 (0%)	6 (29%)
total	4 (0%)	11 (64%)	1 (0%)	5 (0%)	21 (33%)
	1	2	3	4	total

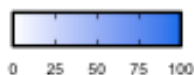
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

6. 6th Place

## Test Set

### Probability Heatmap

	1	2	3	4	Exp
AD	0	80	0	20	2
AE	0	29	0	71	2
AI	2	68	0	30	2
AK	3	71	0	27	2
I	35	20	0	45	2
L	1	7	0	93	2
N	2	70	0	28	2
O	60	39	0	1	2
P	12	76	0	11	2
Q	0	43	0	57	2
S	7	76	0	17	2
V	9	77	0	14	2
W	100	0	0	0	2
Y	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

Model Coefficients

	(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



## Training Set

1	2 (29%)	3 (43%)	0 (0%)	2 (29%)	7 (17%)
2	1 (6%)	12 (75%)	0 (0%)	3 (19%)	16 (39%)
3	0 (0%)	0 (0%)	7 (88%)	1 (12%)	8 (20%)
4	1 (10%)	1 (10%)	1 (10%)	7 (70%)	10 (24%)
total	4 (50%)	16 (75%)	8 (88%)	13 (54%)	41 (68%)
	1	2	3	4	total

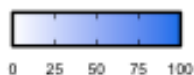
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

7. 7th Place

# Training Set

## Probability Heatmap

	1	2	3	4	Exp
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
AH	15	85	0	0	2
AJ	58	40	0	3	2
G	23	77	0	0	2
J	3	97	0	0	2
K	23	77	0	0	2
M	15	28	0	57	2
T	13	37	0	50	2
U	22	78	0	0	2
X	10	90	0	1	2
AL	8	92	0	0	2
AM	7	93	0	0	2
H	2	39	0	59	2
R	13	87	0	0	2
AO	0	0	93	7	3
AP	0	0	80	19	3
AQ	0	0	97	3	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
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



## Test Set

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	1 (7%)	7 (47%)	3 (20%)	4 (27%)	15 (71%)
3	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
4	0 (0%)	2 (33%)	2 (33%)	2 (33%)	6 (29%)
total	1 (0%)	9 (78%)	5 (0%)	6 (33%)	21 (43%)
	1	2	3	4	total

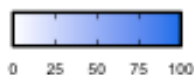
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

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
I	10	79	0	10	2
L	2	8	0	90	2
N	1	1	40	58	2
O	64	22	0	14	2
P	0	0	100	0	2
Q	0	0	100	0	2
S	0	0	98	2	2
V	17	60	0	22	2
W	1	99	0	0	2
Y	7	93	0	0	2
Z	3	97	0	0	2
AV	2	2	33	63	4
AX	3	97	0	0	4
AZ	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 ept)	Total_ P	fr_ester 1	fr_es ter2	fr_hal ogen1	fr_hal ogen2	fr_hal ogen3	fr_halo gen4	fr_hal ogen5	fr_hal 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 (71%)	2 (29%)	0 (0%)	0 (0%)	7 (17%)
2	2 (12%)	12 (75%)	0 (0%)	2 (12%)	16 (39%)
3	0 (0%)	0 (0%)	8 (100%)	0 (0%)	8 (20%)
4	0 (0%)	3 (30%)	0 (0%)	7 (70%)	10 (24%)
total	7 (71%)	17 (71%)	8 (100%)	9 (78%)	41 (78%)
	1	2	3	4	total

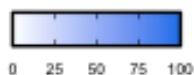
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

8. 8th Place

# Training Set

## Probability Heatmap

	1	2	3	4	Exp
A	16	69	0	15	1
AF	50	8	0	43	1
B	62	35	0	4	1
C	48	46	0	6	1
D	89	11	0	0	1
E	36	55	0	8	1
F	78	14	0	9	1
AA	11	87	0	3	2
AB	0	45	0	55	2
AC	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	2	69	0	28	2
T	83	15	0	1	2
U	0	100	0	0	2
X	11	89	0	0	2
AL	0	100	0	0	2
AM	24	64	0	12	2
H	1	61	0	39	2
R	13	70	0	16	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
AU	0	0	100	0	3
AN	0	0	100	0	3
AW	1	61	0	39	4
AY	0	42	0	58	4
BA	0	39	0	61	4
BB	8	8	0	83	4
BC	8	72	0	20	4
BE	8	8	0	84	4
BH	0	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%)	7 (47%)	5 (33%)	2 (13%)	15 (71%)
3	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
4	0 (0%)	3 (50%)	1 (17%)	2 (33%)	6 (29%)
total	1 (0%)	10 (70%)	6 (0%)	4 (50%)	21 (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

	(Intercept)	NPA_7 _SM	dip_y_ SM	fr_halog en1	fr_halog en2	fr_halog en3	fr_halog en4	fr_halog en5	fr_halog 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 (57%)	2 (29%)	0 (0%)	1 (14%)	7 (17%)
2	0 (0%)	13 (81%)	0 (0%)	3 (19%)	16 (39%)
3	0 (0%)	0 (0%)	8 (100%)	0 (0%)	8 (20%)
4	0 (0%)	3 (30%)	1 (10%)	6 (60%)	10 (24%)
total	4 (100%)	18 (72%)	9 (89%)	10 (60%)	41 (76%)
	1	2	3	4	total

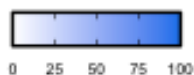
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

9. 9th Place

# Training Set

## Probability Heatmap

	1	2	3	4	Exp
A	10	74	0	17	1
AF	30	15	0	54	1
B	77	23	0	1	1
C	35	63	0	3	1
D	96	4	0	0	1
E	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
T	31	60	0	9	2
U	0	100	0	0	2
X	4	96	0	0	2
AL	0	100	0	0	2
AM	28	67	0	5	2
H	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	0	3
AS	0	0	100	0	3
AT	17	25	34	24	3
AU	0	0	100	0	3
AN	0	0	72	28	3
AW	0	36	0	64	4
AY	0	66	0	34	4
BA	0	25	0	75	4
BB	0	6	0	94	4
BC	6	74	0	20	4
BE	0	3	0	97	4
BH	0	0	28	72	4
BI	3	13	66	18	4
BJ	36	5	0	59	4
BK	0	78	0	22	4



## Test Set

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	5 (33%)	3 (20%)	2 (13%)	5 (33%)	15 (71%)
3	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
4	3 (50%)	1 (17%)	1 (17%)	1 (17%)	6 (29%)
total	8 (0%)	4 (75%)	3 (0%)	6 (17%)	21 (19%)
	1	2	3	4	total

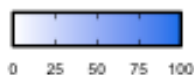
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

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
I	0	5	0	95	2
L	0	7	0	93	2
N	79	19	0	2	2
O	0	0	100	0	2
P	100	0	0	0	2
Q	100	0	0	0	2
S	24	73	0	3	2
V	9	78	0	12	2
W	0	14	0	85	2
Y	0	7	75	17	2
Z	1	6	0	93	2
AV	100	0	0	0	4
AX	1	11	0	88	4
AZ	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									
	(Intercept)	dip_y_P	para_P	fr_halo_gen1	fr_halo_gen2	fr_halo_gen3	fr_halogen4	fr_halo_gen5	fr_halo_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	08	112.25	00	298.464	59	81.813
	49				15		9422		97

## Training Set

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

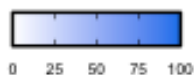
■ Accuracy 
 ■ False 
 ■ Precision 
 ■ Size 
 ■ True

10. 10th Place

# Training Set

## Probability Heatmap

	1	2	3	4	Exp
A	3	40	0	57	1
AF	48	25	0	27	1
B	34	62	0	4	1
C	53	46	0	1	1
D	76	24	0	0	1
E	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
AH	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
T	14	45	0	41	2
U	0	100	0	0	2
X	24	76	0	0	2
AL	0	100	0	0	2
AM	24	68	0	8	2
H	3	56	0	41	2
R	39	58	0	2	2
AO	0	0	100	0	3
AP	0	0	100	0	3
AQ	0	0	97	3	3
AR	0	0	100	0	3
AS	0	0	100	0	3
AT	0	0	100	0	3
AU	0	0	100	0	3
AN	0	0	100	0	3
AW	3	56	0	41	4
AY	0	66	0	34	4
BA	0	6	0	94	4
BB	0	2	3	94	4
BC	11	69	0	20	4
BE	0	1	1	99	4
BH	0	0	0	100	4
BI	8	19	0	73	4
BJ	15	21	0	64	4
BK	14	68	0	18	4





## Test Set

1	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
2	6 (40%)	6 (40%)	2 (13%)	1 (7%)	15 (71%)
3	0 (0%)	0 (0%)	0 (0%)	0 (0%)	0 (0%)
4	1 (17%)	3 (50%)	1 (17%)	1 (17%)	6 (29%)
total	7 (0%)	9 (67%)	3 (0%)	2 (50%)	21 (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
AI	6	58	0	35	2
AK	8	65	0	28	2
I	38	28	0	34	2
L	0	1	85	14	2
N	25	69	0	5	2
O	86	13	0	0	2
P	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
Y	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

