Aldehyde Deuteration - Model Search - Non-ordinal

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Model Search

formula	McFadden R2
class \sim -2-3- + dip_x + dip_y + NPA_1	0.716
class \sim -2-3- + dip_x + dip_y + diff 1 2	0.707
class $\sim \text{dip}_x + \text{dip}_y + \text{Dist}(2, 3) + \text{NPA}_1$	0.699
class $\sim dip_x + dip_y + Dist(2, 3) + diff 1 2$	0.699
class \sim dip_x + dip_y + NPA_1 + NPA_3	0.699
class \sim dip_x + dip_y + NPA_3 + diff 1 2	0.690
class \sim Total + NPA_1 + NPA_3 + loc.B5	0.687
class \sim Total + NPA_3 + diff 1 2 + loc.B5	0.678
class \sim Total + diff 1 2 + diff 2 3 + loc.B5	0.672
class \sim dip_x + dip_y + NPA_1 + diff 1 2	0.671

Section Results Summary

	Training Accuracy	Test Accuracy
1. 1st Place	85.71	92.3
2. 2nd Place	83.33	84.6
3. 3rd Place	88.10	92.3
4. 4th Place	85.71	84.6
5. 5th Place	92.86	84.6

	Training Accuracy	Test Accuracy
6. 6th Place	92.86	84.6
7. 7th Place	85.71	92.3
8.8th Place	85.71	92.3
9.9th Place	88.10	92.3
10. 10th Place	85.71	84.6

1st Place

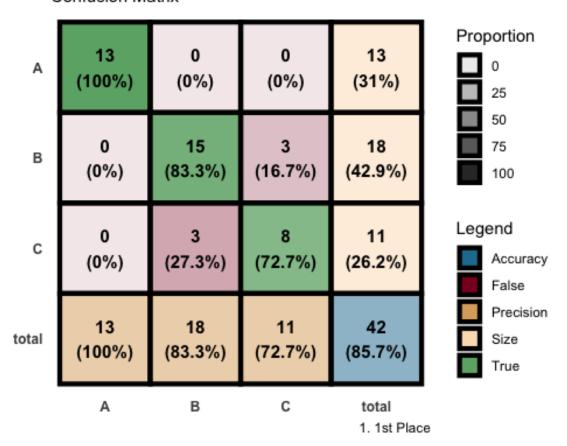
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

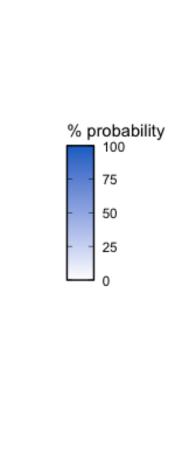
Accuracy McFadden_R2 85.71% 0.716

	(Intercept)	-2-3-	dip_x	dip_y	NPA_1
2	-231.4548	0.1184213	-11.96237	-17.85471	208.7282
3	255.8387	-0.1478514	-11.63987	-18.64964	221.9646

Training Set Confusion Matrix



	Α	В	С
2A	48	44	8
2G	100	0	0
2H	100	0	0
2L	100	0	0
2M	100	0	0
20	100	0	0
2R	92	7	1
2S	93	7	0
2T	100	0	0
2U	100	0	0
2V	100	0	0
2J	100	0	0
2P	100	0	0
2Y	0	81	19
2Z	0	44	56
2AA	0	37	63
2AE	0	96	4
2AF	0	99	1
2AG	0	98	2
2AH	0	96	4
2AJ	0	68	32
2AK	0	92	8
2AM	0	87	13
2AO	0	99 70	1
2W	8	70	22
2X	0	71	29
2AB	0	74	26
2AC	0	70	30
2AP	0	88	12
2AQ	0	99	1
2AR	0	39	61
2AS	0	56	44
2AT	0	31	69
2AU	41	48	11
2AV	0	34	66
2AW	18	64	18
2AX	0	35	65
2AY	0	32	68
2AZ	0	17	83
2BA	0	0	100
2BB	0	17	83
2BC	0	1	99



Exp

В

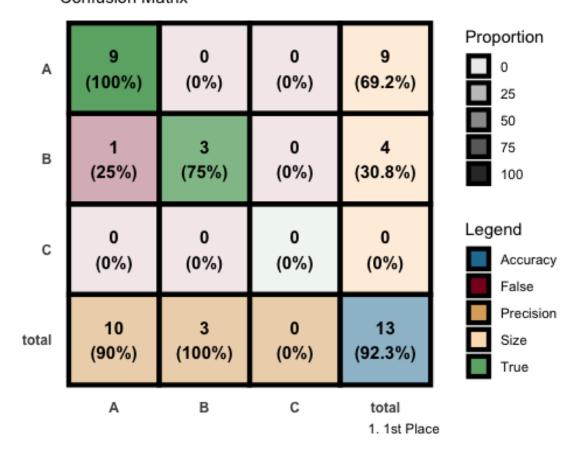
В

В

B B B

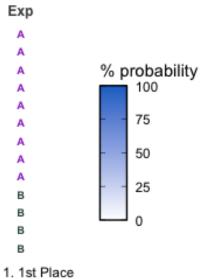
С

Test Set Confusion Matrix

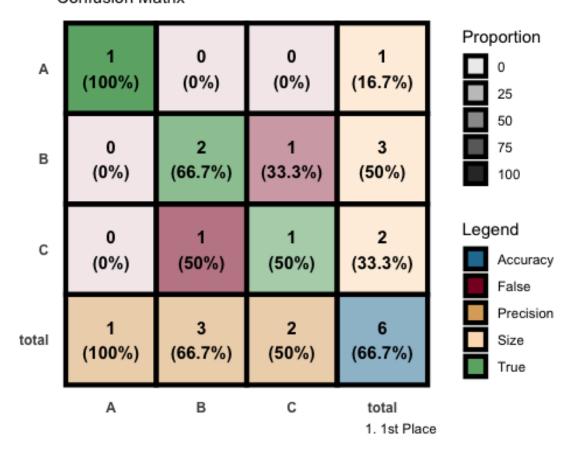


Test Set Probability Heatmap

	Α	В	C
2B	100	0	0
2C	100	0	0
2D	100	0	0
2E	100	0	0
2F	100	0	0
21	100	0	0
2K	100	0	0
2N	100	0	0
2Q	100	0	0
2AD	92	6	2
2AI	0	91	9
2AL	43	56	1
2AN	0	93	7

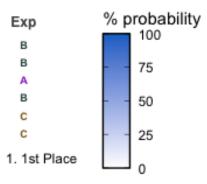


External Validation Confusion Matrix



Probability I	Heatmap
---------------	---------

	A	В	C
2BD	0	98	3
2BE	0	9	91
2BF	100	0	0
2BG	0	88	12
2BH	0	3	97
2BI	0	62	38



2nd Place

Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

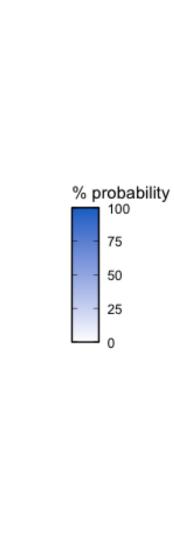
Accuracy McFadden_R2 83.33% 0.707

	(Intercept)	-2-3-	dip_x	dip_y	diff 1 2
2	-285.5935	0.1937231	-11.55657	-17.63469	-201.2935
3	327.8016	-0.1380863	-11.03687	-18.45009	-215.1336

Training Set Confusion Matrix



	Α	В	С
2A	35	55	10
2G	100	0	0
2H	100	0	0
2L	100	0	0
2M	100	0	0
20	100	0	0
2R	91	8	1
2S	92	8	0
2T	100	0	0
2U	100	0	0
2V	100	0	0
2J	100	0	0
2P	100	0	0
2Y	0	84	16
2Z	0	42	58
2AA	0	34	66
2AE	0	98	2
2AF	0	100	0
2AG	0	100	0
2AH	0	98	2
2AJ	0	69	31
2AK	0	95	5
2AM	0	90	10
2AO	0	100 70	0
2W	7	70	23
2X	0	69	31
2AB	0	76	24
2AC	0	69	31
2AP	0	91	9
2AQ	0	100	0
2AR	0	35	65
2AS	0	53	47
2AT	0	27	73
2AU	41	48	10
2AV	0	30	70
2AW	34	52	14
2AX	0	43	57
2AY	0	27	73
2AZ	0	14	86
2BA	0	0	100
2BB	0	13	87
2BC	0	0	100



В

В

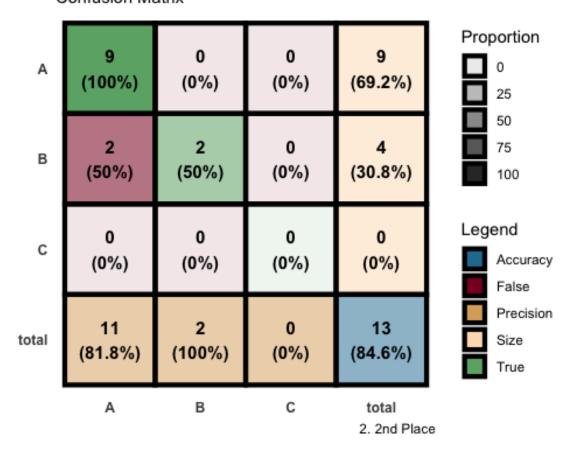
B B B

Exp

2. 2nd Place

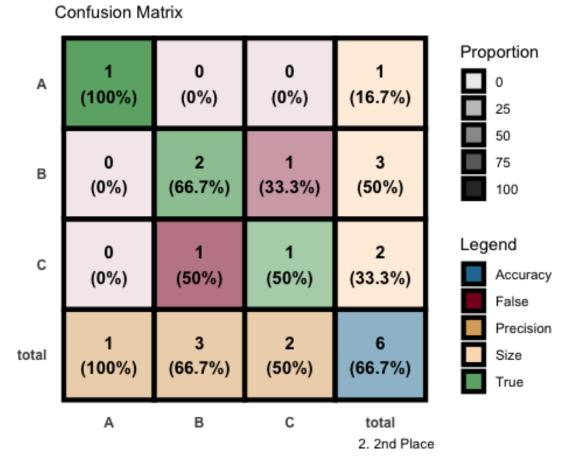
С

Test Set Confusion Matrix



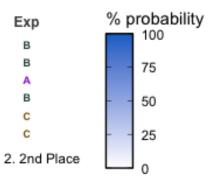
Test Set Probability Heatmap

	Α	В	С	Exp	
2B	100	0	0	A	
2C	100	0	0	A	
2D	100	0	0	A	% probability
2E	100	0	0	A	100
2F	100	0	0	A	
21	100	0	0	A	75
2K	100	0	0	A	50
2N	100	0	0	A	50
2Q	100	0	0	Α	25
2AD	87	9	4	В	[] 25
2AI	0	95	5	В	
2AL	53	46	0	В	O
2AN	0	97	3	В	
				2. 2nd Place	



External Validation Probability Heatmap

A	В	C
0	99	1
0	4	96
100	0	0
0	93	7
0	2	98 34
0	66	34
	0	0 99 0 4 100 0 0 93



3rd Place

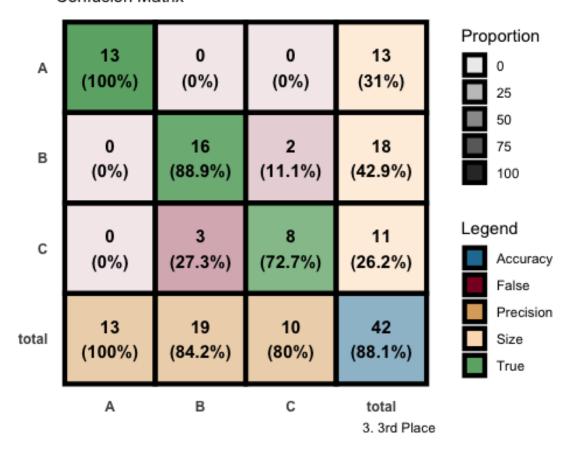
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

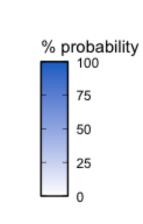
Accuracy McFadden_R2 88.1% 0.699

	(Intercept)	dip_x	dip_y	Dist(2, 3)	NPA_1
2	462.3908	-22.00662	-33.83547	-400.2782	430.6610
3	-465 2533	-21 84399	-34 51954	370 3708	442 1676

Training Set Confusion Matrix



	Α	В	С
2A	72	23	5
2G	100	0	0
2H	100	0	0
2L	100	0	0
2M	100	0	0
20	100	0	0
2R	96	3	1
2S	96	4	0
2T	100	0	0
2U	100	0	0
2V	100	0	0
2J	100	0	0
2P	100	0	0
2Y	0	71	29
2Z	0	46	54
2AA	0	44	56
2AE	0	85	15
2AF	0	95	5
2AG	0	90	10
2AH	0	85	15
2AJ	0	56	44
2AK	0	79	21
2AM	0	84	16
2AO	0	91	9
2W	1	85	15
2X	0	80	20
2AB	0	69	31
2AC	0	72	28
2AP	0	83	17
2AQ	0	91	9
2AR	0	52	48
2AS	0	66	34
2AT	0	43	57
2AU	30	63	7
2AV	0	44	56
2AW	5	65	30
2AX	0	32	68
2AY	0	46	54
2AZ	0	23	77
2BA	0	9	91
2BB	0	19	81
2BC	0	4	96



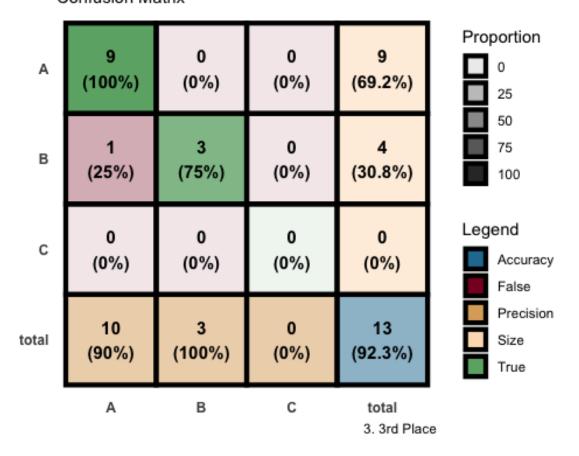
C C

Exp

В

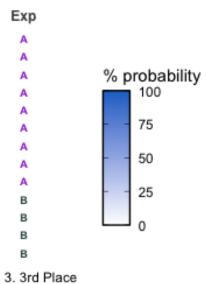
B B

Test Set Confusion Matrix

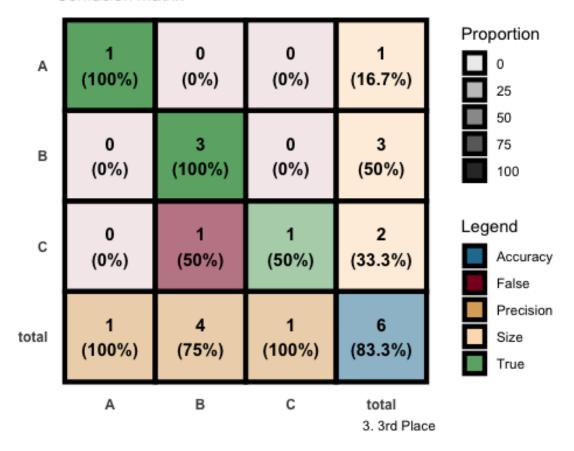


Test Set Probability Heatmap

	Α	В	С
2B	100	0	0
2C	100	0	0
2D	100	0	0
2E	100	0	0
2F	100	0	0
21	100	0	0
2K	100	0	0
2N	100	0	0
2Q	100	0	0
2AD	99	1	0
2AI	0	76	24
2AL	46	50	4
2AN	0	79	21

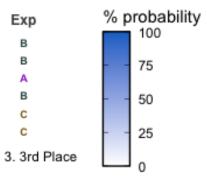


Confusion Matrix



External Validation Probability Heatmap

	A	ь	C
2BD	0	89	11
2BE	0	67	33
2BF	100	0	0
2BG	0	78	22
2BH	0	7	93
2BI	0	50	50



4th Place

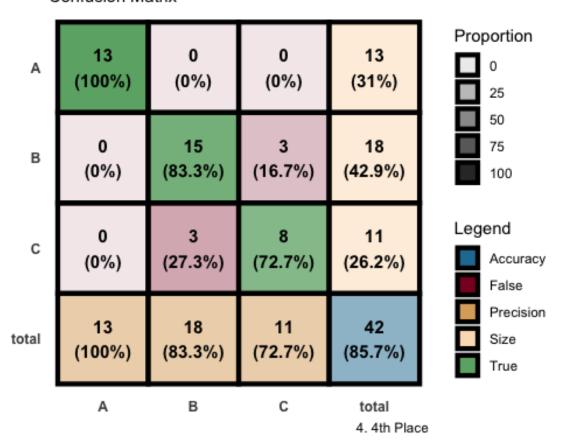
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

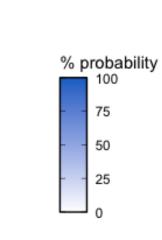
Accuracy McFadden_R2 85.71% 0.699

	(Intercept)	dip_x	dip_y	Dist(2, 3)	diff 1 2
2	661.7346	-22.71409	-36.60076	-398.7258	-475.5286
3	-506.7224	-22.42204	-37.26460	576.4101	-487.2459

Training Set Confusion Matrix



	Α	В	С
2A	60	33	7
2G	100	0	0
2H	100	0	0
2L	100	0	0
2M	100	0	0
20	100	0	0
2R	94	4	2
2S	95	5	0
2T	100	0	0
2U	100	0	0
2V	100	0	0
2J	100	0	0
2P	100	0	0
2Y	0	72	28
2Z	0	43	57
2AA	0	41	59
2AE	0	90	10
2AF	0	98	2 5
2AG	0	95	5
2AH	0	89	11
2AJ	0	54	46
2AK	0	83	17
2AM	0	87	13
2AO	0	95	5
2W	0	86	13
2X	0	80	20 32
2AB	0	68	32
2AC	0	73	27
2AP	0	84	16
2AQ	0	95	5
2AR	0	50	50
2AS	0	63	37
2AT	0	39	61
2AU	30	64	6
2AV	0	40	60
2AW	21	53	26
2AX	0	37	63
2AY	0	42	58
2AZ	0	20	80
2BA	0	3	97
2BB	0	14	86
2BC	0	2	98



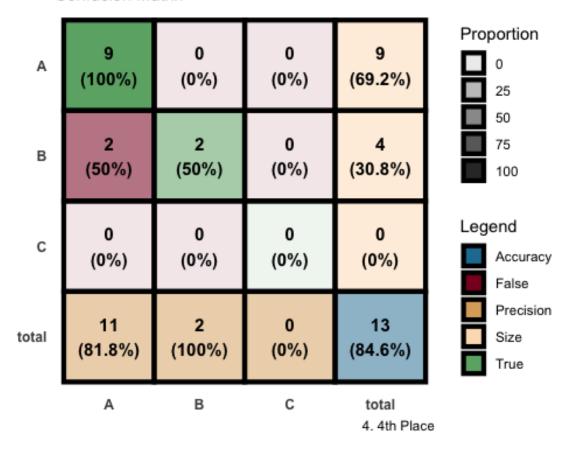
С

Exp

В

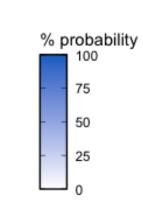
B B B

Test Set Confusion Matrix

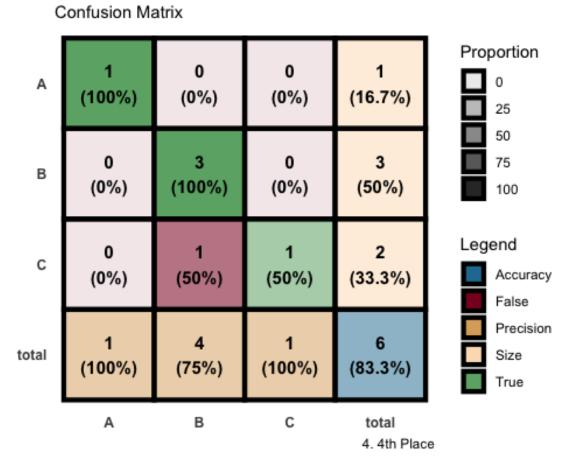


Test Set Probability Heatmap

	Α	В	С	Exp
2B	100	0	0	Α
2C	100	0	0	A
2D	100	0	0	Α
2E	100	0	0	A
2F	100	0	0	A
21	100	0	0	A
2K	100	0	0	Α
2N	100	0	0	Α
2Q	100	0	0	A
2AD	95	4	1	В
2AI	0	81	19	В
2AL	87	12	1	В
2AN	0	85	15	В

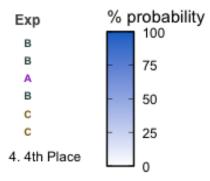


4. 4th Place



External Validation Probability Heatmap

	A	В	C
2BD	0	92	8
2BE	0	64	36
2BF	100	0	0
2BG	0	83	17
2BH	0	5	95
2BI	0	51	49



5th Place

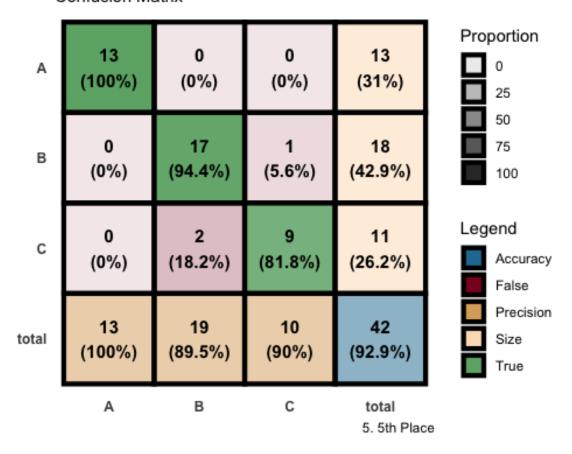
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

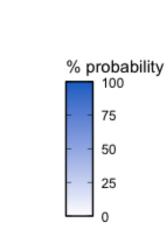
Accuracy McFadden_R2
92.86% 0.699

	(Intercept)	dip_x	dip_y	NPA_1	NPA_3
2	8.19396	-23.17355	-36.01353	461.8364	53.46012
3	-120.57703	-23.06822	-36.08947	481.2963	-201.39613

Training Set Confusion Matrix



	Α	В	С
2A	73	26	1
2G	100	0	0
2H	100	0	0
2L	100	0	0
2M	100	0	0
20	100	0	0
2R	96	3	1
2S	96	4	0
2T	100	0	0
2U	100	0	0
2V	100	0	0
2J	100	0	0
2P	100	0	0
2Y	0	81	19
2Z	0	66	34
2AA	0	52	48
2AE	0	78	22
2AF	0	87	13
2AG	0	91	9
2AH	0	82	18
2AJ	0	26	74
2AK	0	65	35
2AM	0	88	12
2AO	0	91	9
2W	0	97	3
2X	0	96	4
2AB	0	70	30
2AC	0	96	4
2AP	0	93	7
2AQ	0	91	9
2AR	0	60	40
2AS	0	47	53
2AT	0	46	54
2AU	31	67	1
2AV	0	43	57
2AW 2AX	3 0	31 41	67 59
2AY	0	56	44
2AZ	0	8	92
2BA	0	11	89
2BB	0	8	92
2BC	0	1	99
200	U	l l	99



Exp

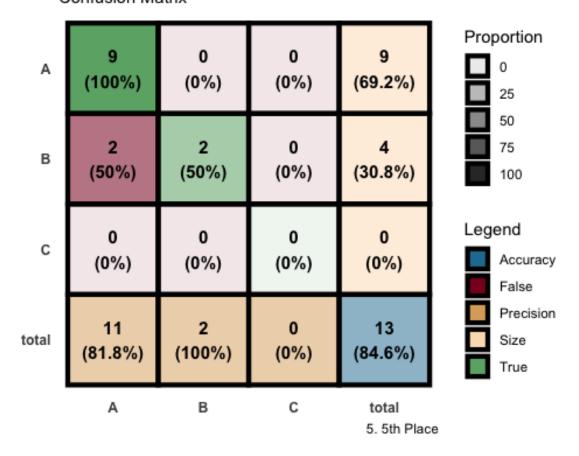
В

B B

5. 5th Place

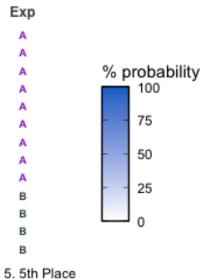
C C

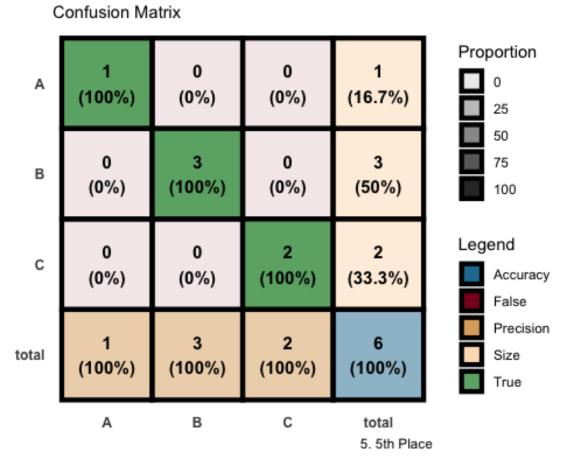
Test Set Confusion Matrix



Test Set Probability Heatmap

	A	В	C
2B	100	0	0
2C	100	0	0
2D	100	0	0
2E	100	0	0
2F	100	0	0
21	100	0	0
2K	100	0	0
2N	100	0	0
2Q	100	0	0
2AD	99	1	0
2AI	0	64	36
2AL	52	44	4
2AN	0	89	11





External Validation Probability Heatmap

	Α	В	С
2BD	0	84	16
2BE	0	85	15
2BF	100	0	0
2BG	0	60	40
2BH	0	2	98
2BI	0	35	65

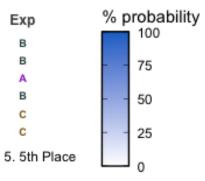


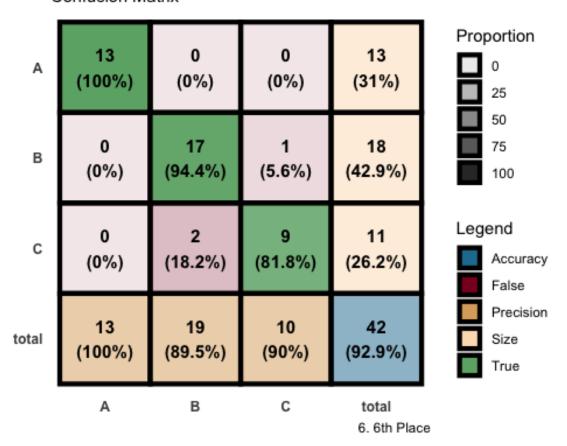
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

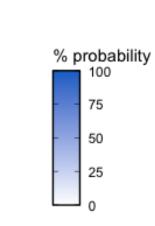
Accuracy McFadden_R2
92.86% 0.69

	(Intercept)	dip_x	dip_y	NPA_3	diff 1 2
2	98.88628	-15.09258	-24.06615	-37.06308	-309.6037
3	-18.63993	-14.97356	-24.24109	-285.15931	-328.8158

Training Set Confusion Matrix



	Α	В	С
2A	56	43	1
2G	100	0	0
2H	100	0	0
2L	100	0	0
2M	100	0	0
20	100	0	0
2R	94	5	1
2S	94	6	0
2T	100	0	0
2U	100	0	0
2V	100	0	0
2J	100	0	0
2P	100	0	0
2Y	0	79	21
2Z	0	64	36
2AA	0	51	49
2AE	0	79	21
2AF	0	89	11
2AG	0	91	9
2AH	0	83	17
2AJ	0	27 66	73
2AK	0	66	34
2AM	0	89	11
2A0	0	91	9
2W	2	95	3
2X	0	95	5
2AB	0	71	29
2AC	0	95	5 7
2AP	0	93	
2AQ	0	91	9
2AR 2AS	0	60	40
2AT	0	46 45	54 55
2AU	46	53	1
2AV	0	43	57
2AW	8	31	61
2AX	0	41	59
2AY	0	56	44
2AZ	0	8	92
2BA	Ö	6	94
2BB	Ö	5	95
2BC	0	1	99

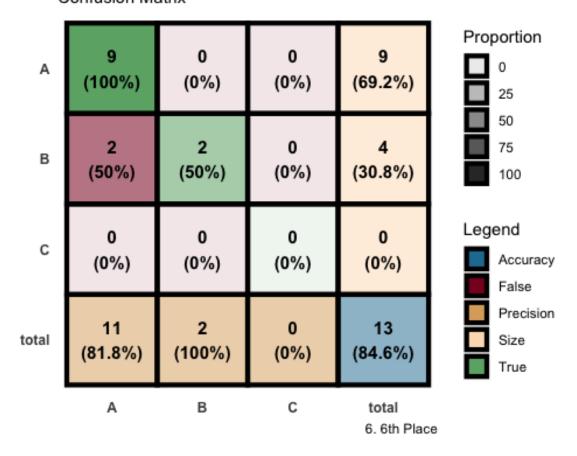


С

В

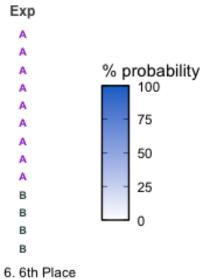
Exp

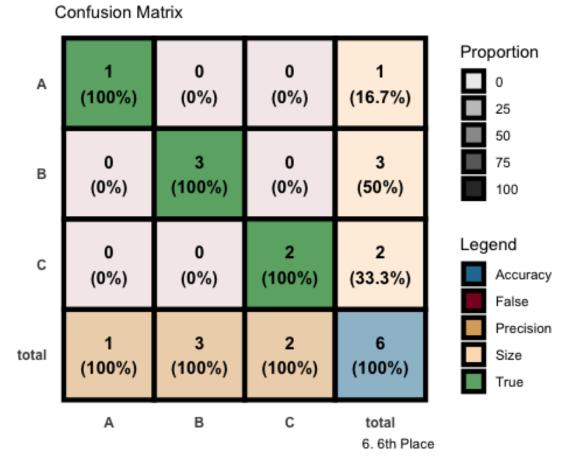
Test Set Confusion Matrix



Test Set Probability Heatmap

	Α	В	С
2B	100	0	0
2C	100	0	0
2D	100	0	0
2E	100	0	0
2F	100	0	0
21	100	0	0
2K	100	0	0
2N	100	0	0
2Q	100	0	0
2AD	90	10	0
2AI	0	66	34
2AL	85	14	1
2AN	0	88	12





Probability Heatmap

	Α	В	C
2BD	0	86	14
2BE	0	83	17
2BF	100	0	0
2BG	0	62	38
2BH	0	2	98
2BI	0	35	65

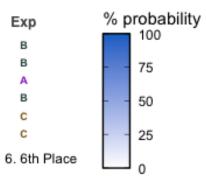


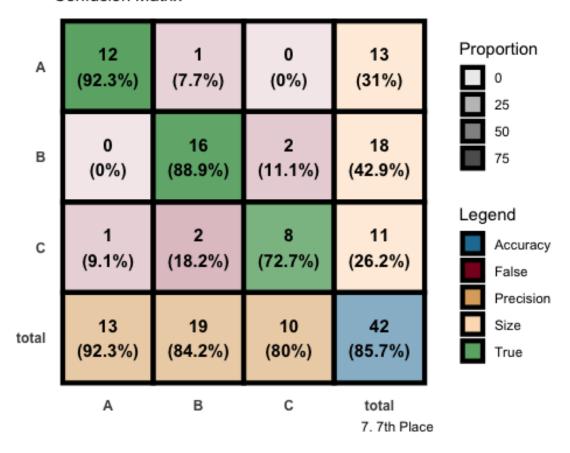
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

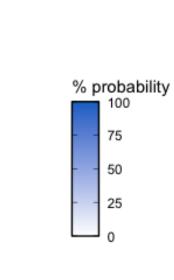
Accuracy McFadden_R2 85.71% 0.687

	(Intercept)	Total	NPA_1	NPA_3	loc.B5
2	-227.6700	13.29595	134.6280	-434.2698	-2.661891
3	-339.3368	13.62434	149.4287	-654.3205	-3.123991

Training Set Confusion Matrix



	Α	В	С
2A	38	59	3
2G	100	0	0
2H	100	0	0
2L	100	0	0
2M	100	0	0
20	100	0	0
2R	89	11	0
2S	82	18	0
2T	100	0	0
2U	100	0	0
2V	100	0	0
2J	100	0	0
2P	100	0	0
2Y	0	67	33
2Z	0	50	50
2AA	0	29	71
2AE	0	84	16 7
2AF	0	93	7
2AG	0	98	2
2AH	1	92	2 8
2AJ	0	50	50
2AK	0	79	21
2AM	0	87	13
2AO	11	89	0
2W	10	86	4
2X	2	91	7
2AB	0	68	32
2AC	0	96	4
2AP	0	91	9
2AQ	0	100	0
2AR	0	57	43
2AS	0	24	76
2AT	0	31	69
2AU	57	41	2
2AV	0	22	78
2AW	9	54	37
2AX	0	35	65
2AY	0	55	45
2AZ	0	30	70
2BA	0		94
2BB	0	6 7	93
2BC	0	1	99



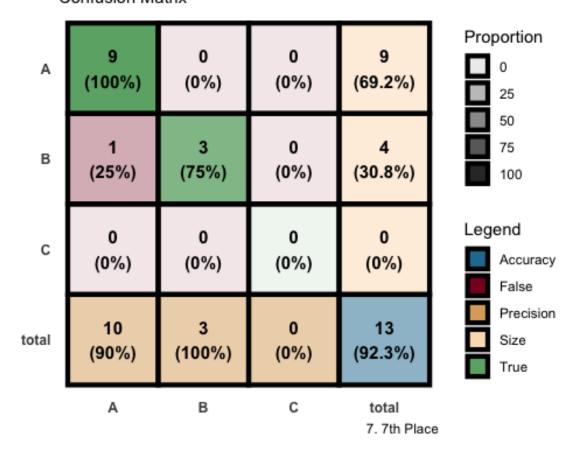
Exp

7. 7th Place

С

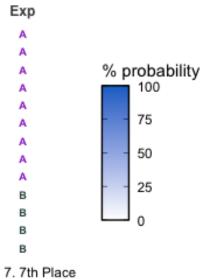
B B

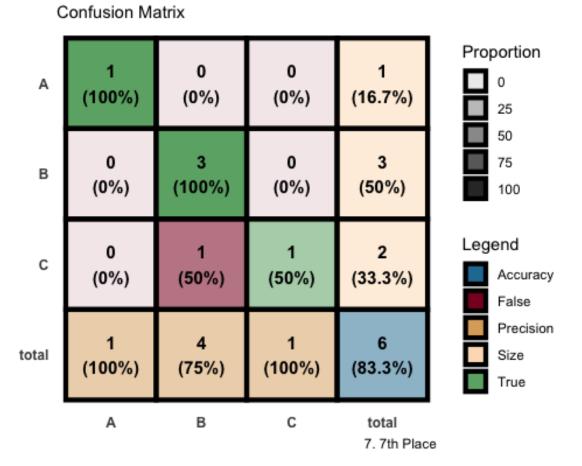
Test Set Confusion Matrix



Test Set Probability Heatmap

	Α	В	С
2B	100	0	0
2C	100	0	0
2D	100	0	0
2E	100	0	0
2F	100	0	0
21	100	0	0
2K	100	0	0
2N	100	0	0
2Q	100	0	0
2AD	6	87	7
2AI	0	89	11
2AL	100	0	0
2AN	0	97	3





External Validation Probability Heatmap

	^	ь	0
2BD	3	89	8
2BE	0	68	32
2BF	100	0	0
2BG	0	85	15
2BH	0	4	96
2BI	0	71	29

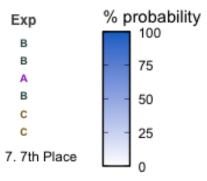


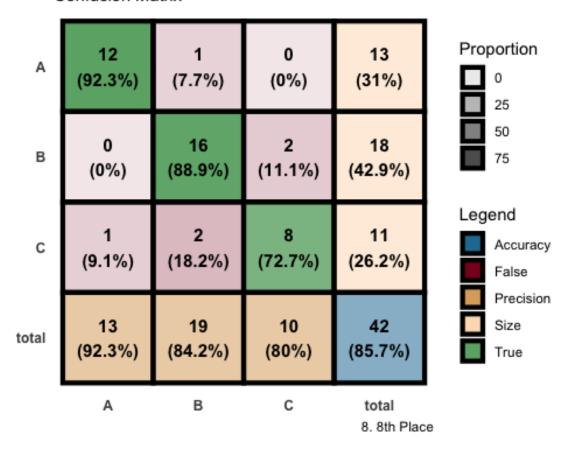
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

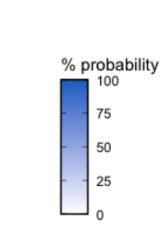
Accuracy McFadden_R2 85.71% 0.678

	(Intercept)	Total	NPA_3	diff 1 2	loc.B5
2	-152.6517	10.99773	-377.3616	-108.4889	-2.136966
3	-255.7061	11.31747	-591.6304	-122.4150	-2.558339

Training Set Confusion Matrix



	Α	В	С
2A	32	64	4
2G	100	0	0
2H	100	0	0
2L	100	0	0
2M	100	0	0
20	100	0	0
2R	84	16	0
2S	79	20	0
2T	100	0	0
2U	100	0	0
2V	100	0	0
2J	100	0	0
2P	100	0	0
2Y	0	67	33
2Z	0	50	50
2AA	0	30	70
2AE	0	84	16
2AF	0	92	7
2AG	0	98	2
2AH	2	90	2 8
2AJ	0	50	50
2AK	0	79	21
2AM	1	87	13
2AO	15	84	0
2W	13	82	5 7
2X	3	90	7
2AB	0	68	32
2AC	0	96	4
2AP	0	90	10
2AQ	0	99	0
2AR	0	57 25	43
2AS	0	25	75
2AT	0	31	69
2AU	57	41	2
2AV	0	23	77
2AW	12	52	36
2AX	0	37	63
2AY	0	55	45
2AZ	0	30	70
2BA	0	5	95
2BB	0	6	94
2BC	0	1	99



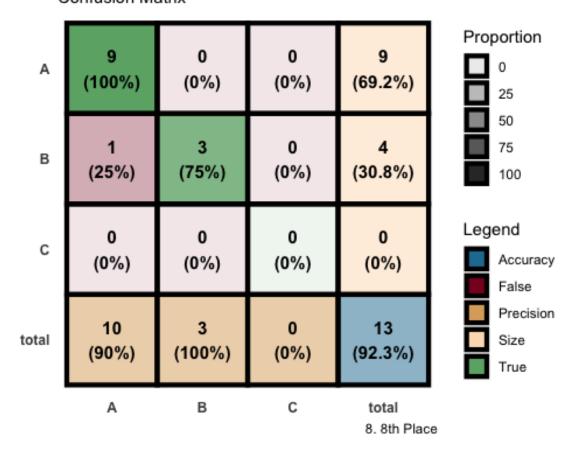
8. 8th Place

С

В

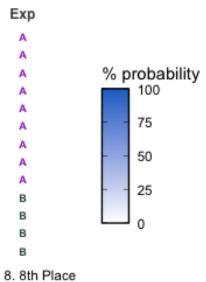
Exp

Test Set Confusion Matrix

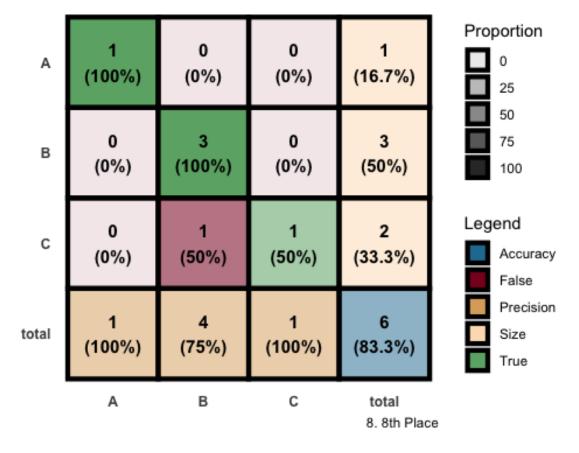


Test Set Probability Heatmap

	A	В	C
2B	100	0	0
2C	100	0	0
2D	100	0	0
2E	100	0	0
2F	100	0	0
21	100	0	0
2K	100	0	0
2N	100	0	0
2Q	100	0	0
2AD	8	85	7
2AI	0	88	11
2AL	100	0	0
2AN	0	96	3



Confusion Matrix



Probability	Heatmap
-------------	---------

	A	В	C
2BD	8	84	8
2BE	0	67	33
2BF	100	0	0
2BG	0	83	17
2BH	0	4	96
2BI	0	71	29

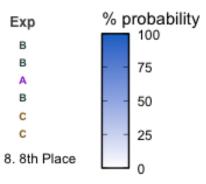


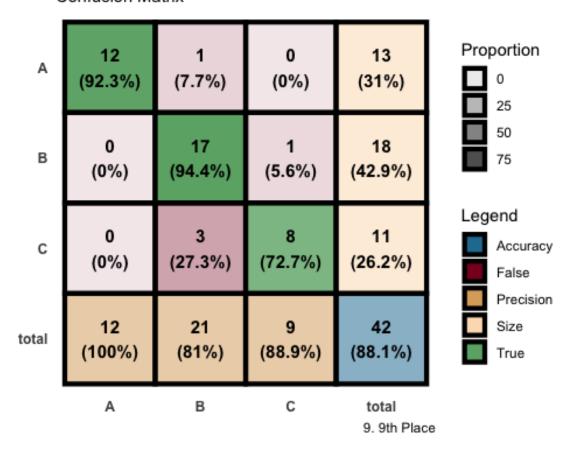
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

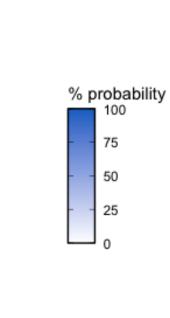
Accuracy McFadden_R2 88.1% 0.672

	(Intercept)	Total	diff 1 2	diff 2 3	loc.B5
2	-329.4002	13.23035	-136.3753	410.1141	-2.819057
3	-443.3563	14.33282	-159.1235	543.2315	-3.494759

Training Set Confusion Matrix



	Α	В	С
2A	48	50	3
2G	100	0	0
2H	100	0	0
2L	100	0	0
2M	100	0	0
20	100	0	0
2R	91	9	0
2S	84	15	1
2T	100	0	0
2U	100	0	0
2V	100	0	0
2J	100	0	0
2P	100	0	0
2Y	0	54	46
2Z	0	53	47
2AA	0	28	72
2AE	0	70	30
2AF	0	84	16
2AG	0	96	4
2AH	0	89	10
2AJ	0	67	33 25
2AK	0	75	25
2AM	0	77	23
2AO	10	90	0
2W	9	84	7
2X	2	89	9
2AB	0	74	26
2AC	0	91	9
2AP	0	90	9
2AQ	0	99	0
2AR	0	55	45
2AS	0	35	65
2AT	0	36	64
2AU	48	49	3
2AV	0	23	77
2AW	7	23 77	16
2AX	0	7	93
2AY	0	52	48
2AZ	0	40	60
2BA	0	14	86
2BB	0	20	80
2BC	0	7	93



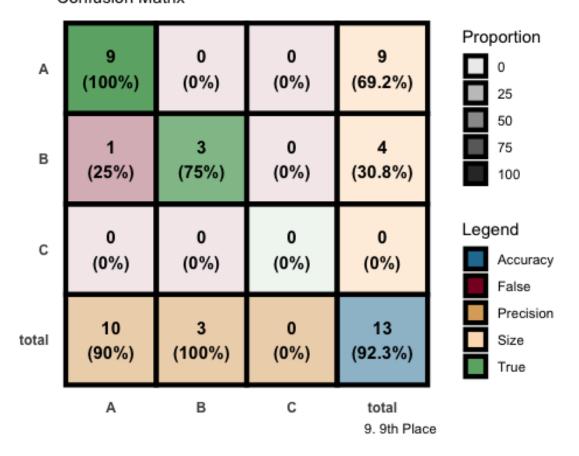
Exp

В

B B B

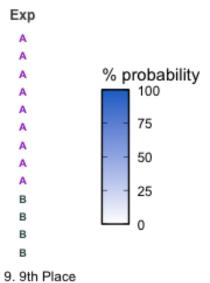
С

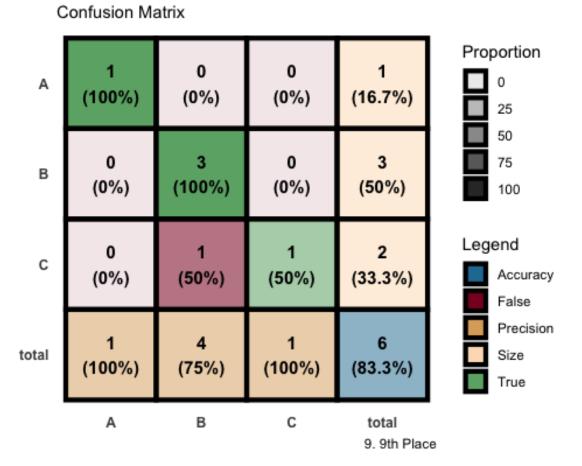
Test Set Confusion Matrix



Test Set Probability Heatmap

	Α	В	C
2B	100	0	0
2C	100	0	0
2D	100	0	0
2E	100	0	0
2F	100	0	0
21	100	0	0
2K	100	0	0
2N	100	0	0
2Q	100	0	0
2AD	8	84	8
2AI	0	90	10
2AL	100	0	0
2AN	0	92	8





Probability Heatmap

	~	ь	C	
2BD	1	88	11	
2BE	0	80	20	
2BF	100	0	0	
2BG	0	87	13	
2BH	0	5	95 32	
2BI	0	68	32	

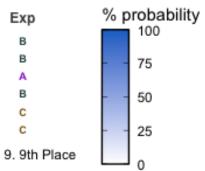


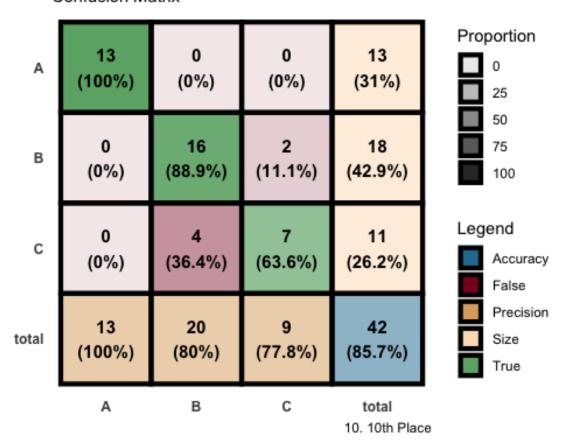
Table:

Full Model Stats - Overall Accuracy and Pseudo-R2

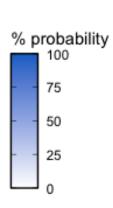
Accuracy McFadden_R2 85.71% 0.671

	(Intercept)	dip_x	dip_y	NPA_1	diff 1 2
2	23.03156	-25.57605	-40.08803	428.3814	-98.56926
3	105.48531	-25.79453	-41.40318	208.4211	-311.07207

Training Set Confusion Matrix



	Α	В	С
2A	71	15	14
2G	100	0	0
2H	100	0	0
2L	100	0	0
2M	100	0	0
20	100	0	0
2R	96	3	1
2S	96	4	0
2T	100	0	0
2U	100	0	0
2V	100	0	0
2J	100	0	0
2P	100	0	0
2Y	0	74	26
2Z	0	26	74
2AA	0	37	63
2AE	0	90	10
2AF	0	98	2
2AG	0	82	18
2AH	0	88	12
2AJ	0	75	25
2AK	0	84	16
2AM	0	96	4
2AO	0	86	14
2W	0	71	29
2X	0	67	33
2AB	0	80	20
2AC	0	50	50
2AP	0	73	27 14
2AQ	0	86	14
2AR	0	78	22
2AS	0	59	41
2AT	0	38	62
2AU	33	51	17
2AV	0	43	57
2AW	4	84	12
2AX	0	42	58
2AY	0	77	23
2AZ	0	32	68
2BA	0	4	96
2BB	0	4	96
2BC	0	4	96



С

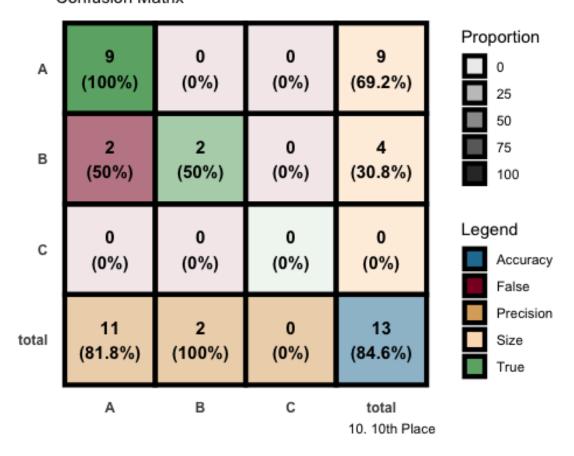
В

В

B B B

Exp

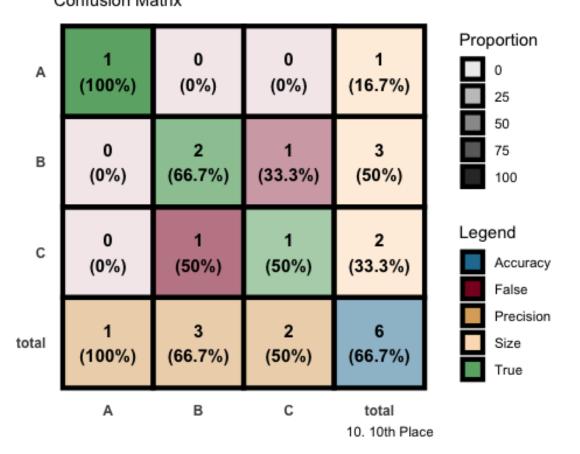
Test Set Confusion Matrix



Test Set Probability Heatmap

	Α	В	С	Exp	
2B	100	0	0	A	
2C	100	0	0	A	
2D	100	0	0	A	% probability
2E	100	0	0	A	100
2F	100	0	0	A	
21	100	0	0	A	75
2K	100	0	0	A	F.0
2N	100	0	0	A	50
2Q	100	0	0	A	25
2AD	99	1	0	В	- 25
2AI	0	83	17	В	
2AL	59	39	2	В	U
2AN	0	73	27	В	
				10. 10th Place	

External Validation Confusion Matrix



Р	Probability Heatmap					
	Α	В	С	Exp	% probability	
2BD	0	92	8	В	100	
2BE	0	27	73	В	75	
2BF	100	0	0	A		
2BG	0	72	28	В	50	
2BH	0	6	94	С		
2BI	0	68	32	С	25	
				10. 10th Place		