Integration of transcriptomics and metabonomics - improving diagnostics, biomarker identification and phenotyping in ulcerative colitis - Supplementary material

April 16, 2013

1 Prediction results -logistic regression fitted by Lasso (i.e. including variable selection)

1.1 ActiveControl

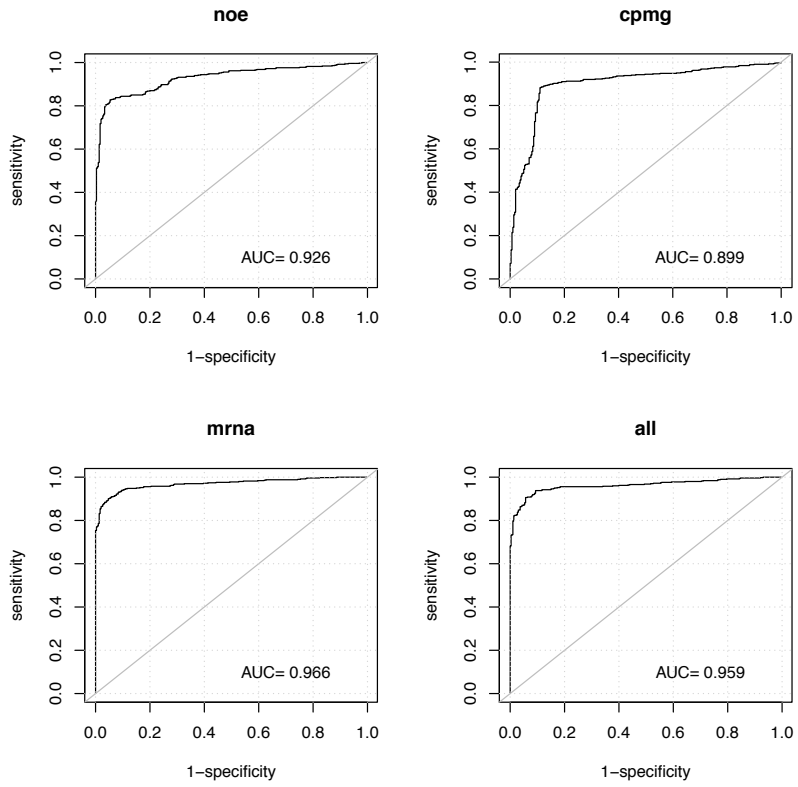

Figure 1: Prediction (logistic regression fitted by lasso) performance for "activeControl" analysis. ROC curves for each data set.

	Name	HGNC	Ppm	Data set	Selection freq.
14301	ENSG00000180616_at	SSTR2		mrna	0.65
11504	ENSG00000165188_at	RNF183		mrna	0.59
10703	ENSG00000162174_at	ASRGL1		mrna	0.5
14514	ENSG00000182240_at	BACE2		mrna	0.39
911	ENSG00000014257_at	ACPP		mrna	0.34
1638	ENSG00000070081_at	NUCB2		mrna	0.33
13932	ENSG00000178078_at	STAP2		mrna	0.32
14507	ENSG00000182199_at	SHMT2		mrna	0.27
5216	ENSG00000118523_at	CTGF		mrna	0.26
15134	ENSG00000185624_at	P4HB		mrna	0.22
9641	ENSG00000152454_at	ZNF256		mrna	0.19

3438	ENSG00000104870_at	FCGRT		mrna	0.18
5339	ENSG00000119777_at	TMEM214		mrna	0.18
12405	ENSG00000169071_at	ROR2		mrna	0.17
936	ENSG00000017483_at	SLC38A5		mrna	0.16
10117	ENSG00000157020_at	SEC13		mrna	0.15
3285	ENSG00000103502_at	CDIPT		mrna	0.14
5651	ENSG00000122585_at	NPY		mrna	0.14
1547	ENSG00000067225_at	PKM2		mrna	0.13
8412	ENSG00000142178_at	SIK1		mrna	0.13
16336	ENSG00000198363_at	ASPH		mrna	0.13
1476	ENSG00000065485_at	PDIA5		mrna	0.12
419	aspartate		2.674261917	noe	0.11
2215	ENSG00000086548_at	CEACAM6		mrna	0.11
4513	ENSG00000112759_at	SLC29A1		mrna	0.11
6405	ENSG00000128918_at	ALDH1A2		mrna	0.11
6472	ENSG00000129538_at	RNASE1		mrna	0.11
9279	ENSG00000148926_at	ADM		mrna	0.11

Table 1: selected variables (active control, combined data set)

	Name	HGNC	Selection freq.
13737	ENSG00000180616_at	SSTR2	0.58
10139	ENSG00000162174_at	ASRGL1	0.55
10940	ENSG00000165188_at	RNF183	0.55
347	ENSG00000014257_at	ACPP	0.39
1074	ENSG00000070081_at	NUCB2	0.38
13368	ENSG00000178078_at	STAP2	0.36
14570	ENSG00000185624_at	P4HB	0.32
13950	ENSG00000182240_at	BACE2	0.27
4992	ENSG00000121690_at	DEPDC7	0.22
4652	ENSG00000118523_at	CTGF	0.2
13943	ENSG00000182199_at	SHMT2	0.2
15772	ENSG00000198363_at	ASPH	0.17
2874	ENSG00000104870_at	FCGRT	0.16
5087	ENSG00000122585_at	NPY	0.14
372	ENSG00000017483_at	SLC38A5	0.13
9077	ENSG00000152454_at	ZNF256	0.12

Table 2: selected variables (active control, mrna data set)

	Name	Ppm	Selection freq.
97	gpc	3.225218334	0.96
100	taurine	3.252754895	0.77
74	aspartate	2.674261917	0.68
98		3.239711261	0.51
80		2.828531781	0.37
73		2.657284529	0.35
63	glutathione	2.533525729	0.32
77	aspartate	2.78947264	0.27
107		3.612395741	0.23
4		0.920966247	0.18
102		3.280717718	0.18
106		3.592624177	0.15
11	valine	0.987778095	0.13
16	lipid	1.281397504	0.12

Table 3: selected variables (active control, noe data set)

	Name	Ppm	Selection freq.
173	gpc	3.225067352	0.78
191		3.68024848	0.74
176	taurine	3.252896929	0.7
275		4.656456115	0.47
192		3.689158497	0.21
174		3.240746725	0.18
4	isoleucine	0.92261137	0.16
86	glutamate	2.333058477	0.14
128	aspartate	2.786412373	0.14

Table 4: selected variables (active control, cpgm data set)

1.2 InactiveActive

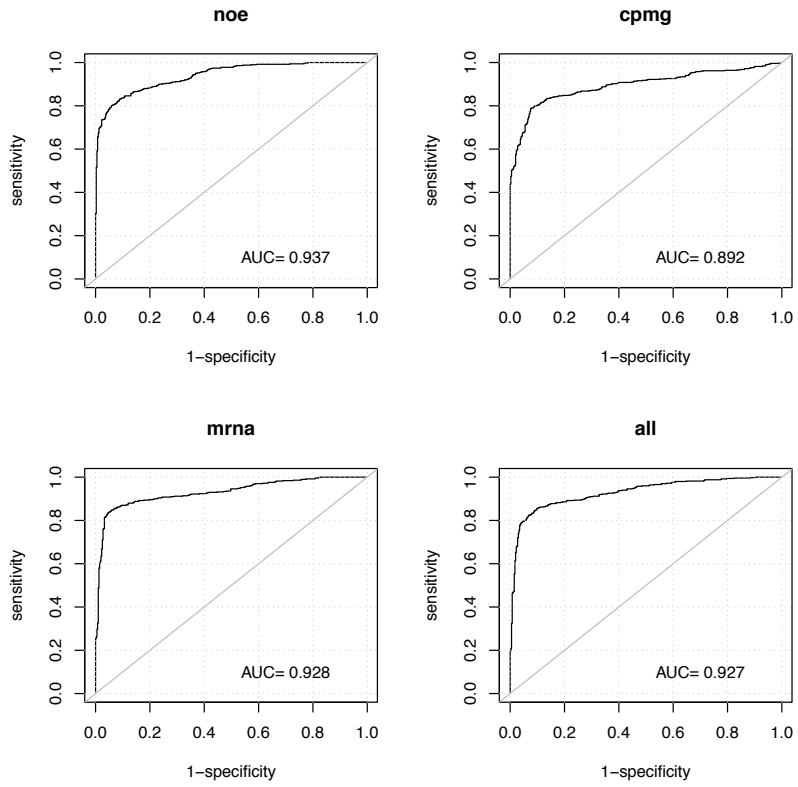

Figure 2: Prediction (logistic regression fitted by lasso) performance for "InactiveActive" analysis. ROC curves for each data set.

	Name	HGNC	Ppm	Data set	Selection freq.
19736	ENSG00000257512_at			mrna	0.55
12663	ENSG00000170419_at	VSTM2A		mrna	0.47
3550	ENSG00000105404_at	RABAC1		mrna	0.4
1325	ENSG00000057704_at	TMCC3		mrna	0.37
1950	ENSG00000078401_at	EDN1		mrna	0.37
15907	ENSG00000196660_at	SLC30A10		mrna	0.37
7251	ENSG00000134910_at	STT3A		mrna	0.36
6715	ENSG00000131174_at	COX7B		mrna	0.34
15147	ENSG00000185670_at	ZBTB3		mrna	0.34
13007	ENSG00000172023_at	REG1B		mrna	0.33
4239	ENSG00000110799_at	VWF		mrna	0.29

652	ENSG00000005238_at	KIAA1539		mrna	0.24
4536	ENSG00000112977_at	DAP		mrna	0.23
8888	ENSG00000145675_at	PIK3R1		mrna	0.23
10858	ENSG00000162909_at	CAPN2		mrna	0.22
3030	ENSG00000101665_at	SMAD7		mrna	0.21
5499	ENSG00000120963_at	ZNF706		mrna	0.21
10895	ENSG00000163053_at	SLC16A14		mrna	0.19
16531	ENSG00000198856_at	OSTC		mrna	0.19
202			3.742516185	cpmg	0.18
1067	ENSG00000034533_at	ASTE1		mrna	0.18
8485	ENSG00000142748_at	FCN3		mrna	0.18
2930	ENSG00000101189_at	C20orf20		mrna	0.16
1638	ENSG00000070081_at	NUCB2		mrna	0.15
14514	ENSG00000182240_at	BACE2		mrna	0.15
18908	ENSG00000244038_at	DDOST		mrna	0.15
911	ENSG00000014257_at	ACPP		mrna	0.14
11382	ENSG00000164683_at	HEY1		mrna	0.14
13225	ENSG00000173269_at	MMRN2		mrna	0.14
2918	ENSG00000101150_at	TPD52L2		mrna	0.13
8412	ENSG00000142178_at	SIK1		mrna	0.13
13280	ENSG00000173598_at	NUDT4		mrna	0.11

Table 5: selected variables (inactive active, combined data set)

	Name	HGNC	Selection freq.
19172	ENSG00000257512_at		0.63
15343	ENSG00000196660_at	SLC30A10	0.46
6151	ENSG00000131174_at	COX7B	0.41
6687	ENSG00000134910_at	STT3A	0.39
12099	ENSG00000170419_at	VSTM2A	0.39
2986	ENSG00000105404_at	RABAC1	0.37
12443	ENSG00000172023_at	REG1B	0.37
761	ENSG00000057704_at	TMCC3	0.35
1386	ENSG00000078401_at	EDN1	0.35
88	ENSG00000005238_at	KIAA1539	0.34
10294	ENSG00000162909_at	CAPN2	0.34
4935	ENSG00000120963_at	ZNF706	0.32
7921	ENSG00000142748_at	FCN3	0.28
3972	ENSG00000112977_at	DAP	0.26
14583	ENSG00000185670_at	ZBTB3	0.26

2366	ENSG00000101189_at	C20orf20	0.25
3675	ENSG00000110799_at	VWF	0.25
10331	ENSG00000163053_at	SLC16A14	0.22
8324	ENSG00000145675_at	PIK3R1	0.19
11737	ENSG00000168575_at	SLC20A2	0.17
503	ENSG00000034533_at	ASTE1	0.16
2466	ENSG00000101665_at	SMAD7	0.16
10818	ENSG00000164683_at	HEY1	0.16
13950	ENSG00000182240_at	BACE2	0.16
9553	ENSG00000157020_at	SEC13	0.15
9792	ENSG00000159128_at	IFNGR2	0.14
12896	ENSG00000174807_at	CD248	0.14
15967	ENSG00000198856_at	OSTC	0.14
18344	ENSG00000244038_at	DDOST	0.14
1125	ENSG00000071243_at	ING3	0.13
2382	ENSG00000101224_at	CDC25B	0.13
4344	ENSG00000115963_at	RND3	0.12
9442	ENSG00000156030_at	C14orf43	0.12
11055	ENSG00000165702_at	GFI1B	0.12
12661	ENSG00000173269_at	MMRN2	0.12
9251	ENSG00000154122_at	ANKH	0.11
10766	ENSG00000164442_at	CITED2	0.11
12092	ENSG00000170381_at	SEMA3E	0.11
12716	ENSG00000173598_at	NUDT4	0.11

Table 6: selected variables (inactive active, mrna data set)

	Name	Ppm	Selection freq.
100	taurine	3.252754895	0.85
74	aspartate	2.674261917	0.82
97	gpc	3.225218334	0.69
139	myo-inositol	4.046452197	0.69
98		3.239711261	0.61
116		3.737919525	0.52
112		3.712430882	0.49
191		6.507960949	0.34
103	scyllo-inositol	3.335121944	0.31
113		3.719207131	0.31
14	valine	1.029642612	0.3
138	myo-inositol	4.039501879	0.29

135		4.005477649	0.22
107		3.612395741	0.21
207		8.17223717	0.16
106		3.592624177	0.15
200		7.397806116	0.15
48	lipid	2.253171801	0.14
118		3.750663847	0.14
203		7.869591075	0.14
211		8.253616906	0.14
53	glutamate	2.33901612	0.12

Table 7: selected variables (inactive active, noe data set)

	Name	Ppm	Selection freq.
176	taurine	3.252896929	0.77
183	scyllo-inositol	3.334861322	0.65
202		3.742516185	0.65
79		2.269194746	0.6
173	gpc	3.225067352	0.55
42		1.880897982	0.54
104		2.508036326	0.5
134		2.855230444	0.46
149		3.005623611	0.43
292		5.897989325	0.43
168		3.175844955	0.42
118	aspartate	2.644782678	0.41
83		2.299460478	0.4
178	taurine	3.278200138	0.39
318		7.347346035	0.36
152		3.042576182	0.34
206		3.761894842	0.33
227		3.996872536	0.33
341		8.693240002	0.3
120	aspartate	2.673924337	0.27
293		5.9012133	0.25
169		3.188072049	0.23
338		8.252995481	0.22
281	glucose	5.23140479	0.21
175		3.246623599	0.2
275		4.656456115	0.2

190		3.612459587	0.18
289		5.79678976	0.17
304		6.089434715	0.17
65	glutamine	2.128764526	0.16
196		3.7126113	0.16
255		4.28480121	0.16
286	glycogen	5.424593506	0.15
86	glutamate	2.333058477	0.14
92		2.384329941	0.13
29		1.611793593	0.12
35		1.680144048	0.12
235	myo-inositol	4.046572122	0.12
191		3.68024848	0.11
280	glucose	5.212160888	0.11
323		7.433508139	0.11

Table 8: selected variables (inactive active, cpmg data set)

1.3 InactiveControl

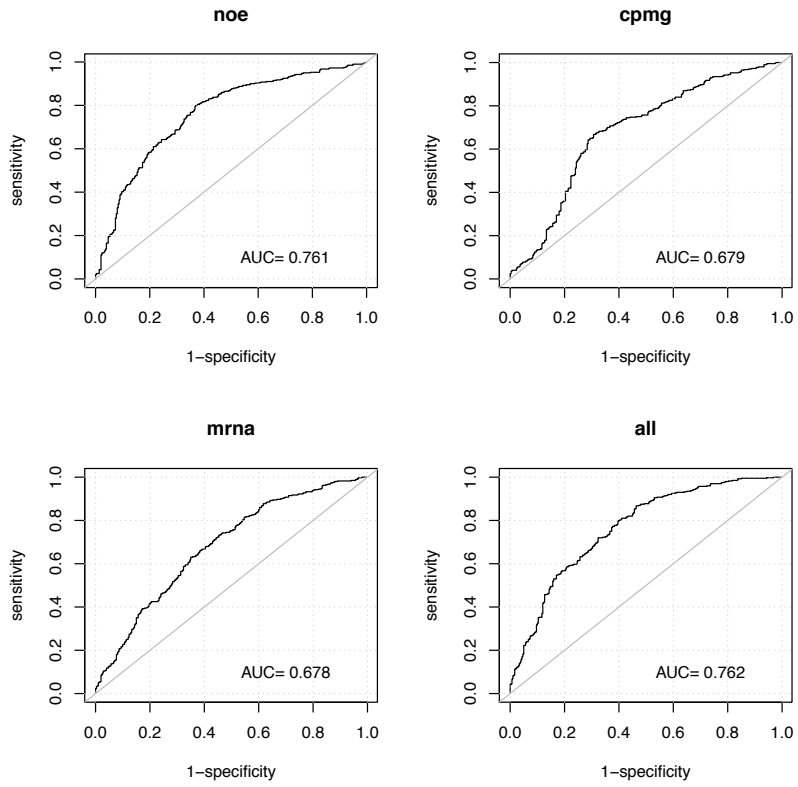

Figure 3: Prediction (logistic regression fitted by lasso) performance for "InactiveControl" analysis. ROC curves for each data set.

	Name	HGNC	Ppm	Data set	Selection freq.
18865	ENSG00000243024_at	RPS11P6		mrna	0.81
168			3.175844955	cpmg	0.77
11605	ENSG00000165669_at	FAM204A		mrna	0.69
5527	ENSG00000121351_at	IAPP		mrna	0.55
5454	ENSG00000120675_at	DNAJC15		mrna	0.5
2845	ENSG00000100664_at	EIF5		mrna	0.48
6400	ENSG00000128881_at	TTBK2		mrna	0.47
5032	ENSG00000116885_at	OSCP1		mrna	0.46
11760	ENSG00000166323_at	C11orf65		mrna	0.31
156			3.092754442	cpmg	0.29
10372	ENSG00000159208_at	C1orf51		mrna	0.29

5293	ENSG00000119487_at	MAPKAP1		mrna	0.27
11284	ENSG00000164291_at	ARSK		mrna	0.26
12952	ENSG00000171786_at	NHLH1		mrna	0.23
16434	ENSG00000198590_at	C3orf35		mrna	0.17
1245	ENSG00000051620_at	HEBP2		mrna	0.15
13574	ENSG00000175550_at	DRAP1		mrna	0.14
5651	ENSG00000122585_at	NPY		mrna	0.13
6774	ENSG00000131697_at	NPHP4		mrna	0.12
425			2.828531781	noe	0.11
4283	ENSG00000111224_at	PARP11		mrna	0.11
15671	ENSG00000189068_at	VSTM1		mrna	0.11
19749	ENSG00000257726_at			mrna	0.11

Table 9: selected variables (inactive control, combined data set)

	Name	HGNC	Selection freq.
18301	ENSG00000243024_at	RPS11P6	0.64
11041	ENSG00000165669_at	FAM204A	0.62
4963	ENSG00000121351_at	IAPP	0.57
2281	ENSG00000100664_at	EIF5	0.53
4890	ENSG00000120675_at	DNAJC15	0.41
4468	ENSG00000116885_at	OSCP1	0.34
9808	ENSG00000159208_at	C1orf51	0.32
4729	ENSG00000119487_at	MAPKAP1	0.22
5836	ENSG00000128881_at	TTBK2	0.21
10720	ENSG00000164291_at	ARSK	0.21
15870	ENSG00000198590_at	C3orf35	0.19
681	ENSG00000051620_at	HEBP2	0.18
5087	ENSG00000122585_at	NPY	0.18
11196	ENSG00000166323_at	C11orf65	0.17
99	ENSG00000005471_at	ABCB4	0.15
6210	ENSG00000131697_at	NPHP4	0.15
12388	ENSG00000171786_at	NHLH1	0.14
15654	ENSG00000197928_at	ZNF677	0.13
12061	ENSG00000170255_at	MRGPRX1	0.11
15277	ENSG00000196440_at	ARMCX4	0.11

Table 10: selected variables (inactive control, mrna data set)

	Name	Ppm	Selection freq.

112		3.712430882	0.84
80		2.828531781	0.82
6		0.943470556	0.73
19	alanine	1.463141868	0.71
61	glutamine	2.448871784	0.65
116		3.737919525	0.58
162		4.477803679	0.52
47		2.196867564	0.45
104		3.347534709	0.36
59	glutamine	2.423782982	0.35
203		7.869591075	0.34
35		2.0960042	0.3
26	acetate	1.91089789	0.29
108		3.688078694	0.28
179		5.90484906	0.28
12		0.998882741	0.27
134	phosphorylethanolamine	3.967780015	0.27
20	alanine	1.478930983	0.23
150		4.245506812	0.22
175	glycogen	5.414940797	0.22
37	glutamine	2.109300297	0.2
69	glutathione	2.579566468	0.2
176	glycogen	5.423161326	0.19
193	tyrosine	6.895575388	0.19
77	aspartate	2.78947264	0.18
15	valine	1.041413537	0.15
118		3.750663847	0.15
38	glutamine	2.115636719	0.13
114		3.726480719	0.13
156		4.353531113	0.13

Table 11: selected variables (inactive control, noe data set)

	Name	Ppm	Selection freq.
168		3.175844955	0.94
266		4.48200363	0.86
156		3.092754442	0.72
196		3.7126113	0.46
102		2.474182837	0.17
75		2.222863533	0.14

23	alanine	1.463121505	0.13
79		2.269194746	0.12

Table 12: selected variables (inactive control, cpmg data set)

1.4 SiSd

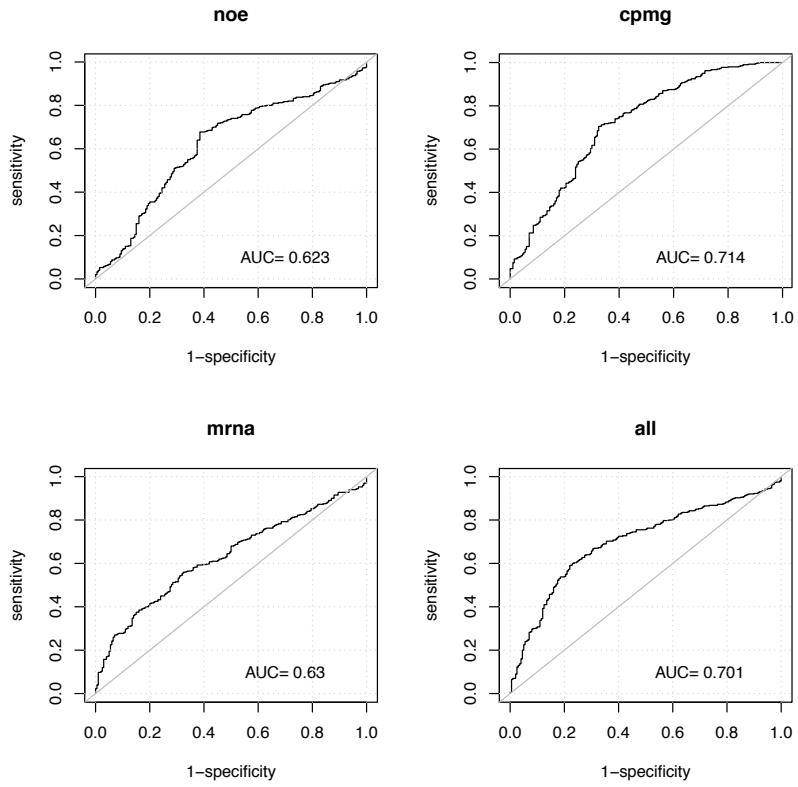

Figure 4: Prediction (logistic regression fitted by lasso) performance for "SiSd" analysis. ROC curves for each data set.

	Name	HGNC	Ppm	Data set	Selection freq.
15124	ENSG00000185565_at	LSAMP		mrna	0.43
180			3.315476883	cpmg	0.39
9280	ENSG00000148935_at	GAS2		mrna	0.37
10339	ENSG00000158874_at	APOA2		mrna	0.24
3506	ENSG00000105229_at	PIAS4		mrna	0.23
1436	ENSG00000064601_at	CTSA		mrna	0.22
3468	ENSG00000104964_at	AES		mrna	0.2
5235	ENSG00000118785_at	SPP1		mrna	0.18
7925	ENSG00000138617_at	PARP16		mrna	0.16
81			2.284443338	cpmg	0.15
8845	ENSG00000145284_at	SCD5		mrna	0.14

15495	ENSG00000188002_at			mrna	0.13
15968	ENSG00000196950_at	SLC39A10		mrna	0.12
276			4.758837295	cpmg	0.11

Table 13: selected variables (SiSd, combined data set)

	Name	HGNC	Selection freq.
14560	ENSG00000185565_at	LSAMP	0.47
8716	ENSG00000148935_at	GAS2	0.32
2942	ENSG00000105229_at	PIAS4	0.26
4671	ENSG00000118785_at	SPP1	0.25
2904	ENSG00000104964_at	AES	0.2
872	ENSG00000064601_at	CTSA	0.18
9775	ENSG00000158874_at	APOA2	0.16
6902	ENSG00000136098_at	NEK3	0.13
10586	ENSG00000163909_at	HEYL	0.13
372	ENSG00000017483_at	SLC38A5	0.11
12705	ENSG00000173557_at	C2orf70	0.11

Table 14: selected variables (SiSd, mrna data set)

	Name	Ppm	Selection freq.
106		3.592624177	0.64
48	lipid	2.253171801	0.53
219		9.471835614	0.5
69	glutathione	2.579566468	0.3
196		7.209519457	0.3
97	gpc	3.225218334	0.28
46		2.178066051	0.27
129		3.936503585	0.27
47		2.196867564	0.26
137		4.022206902	0.26
124		3.804976661	0.25
112		3.712430882	0.21
14	valine	1.029642612	0.2
26	acetate	1.91089789	0.16
57		2.373326067	0.16
192	tyrosine	6.874034118	0.15
21	lipid	1.589194955	0.14
44	glutamine	2.154278502	0.14

45		2.165289332	0.14
60	glutamine	2.436397544	0.14
140	myo-inositol	4.053887421	0.14
162		4.477803679	0.14
170	glucose	5.212423383	0.14
123		3.799400243	0.13
104		3.347534709	0.11

Table 15: selected variables (SiSd, noe data set)

	Name	Ppm	Selection freq.
81		2.284443338	0.86
276		4.758837295	0.73
180		3.315476883	0.51
345		9.475774448	0.48
104		2.508036326	0.35
323		7.433508139	0.34
260		4.35270246	0.32
184		3.346628064	0.31
179		3.296905	0.27
242	lactate	4.111888776	0.27
92		2.384329941	0.25
49		1.983786542	0.24
255		4.28480121	0.19
280	glucose	5.212160888	0.19
314		7.210899163	0.19
227		3.996872536	0.18
158		3.105224973	0.17
48		1.97267515	0.14
73		2.194471652	0.14
190		3.612459587	0.14
234	myo-inositol	4.039315523	0.14
137		2.89984999	0.13
327		7.872866325	0.11

Table 16: selected variables (SiSd, cpmg data set)

1.5 Duration

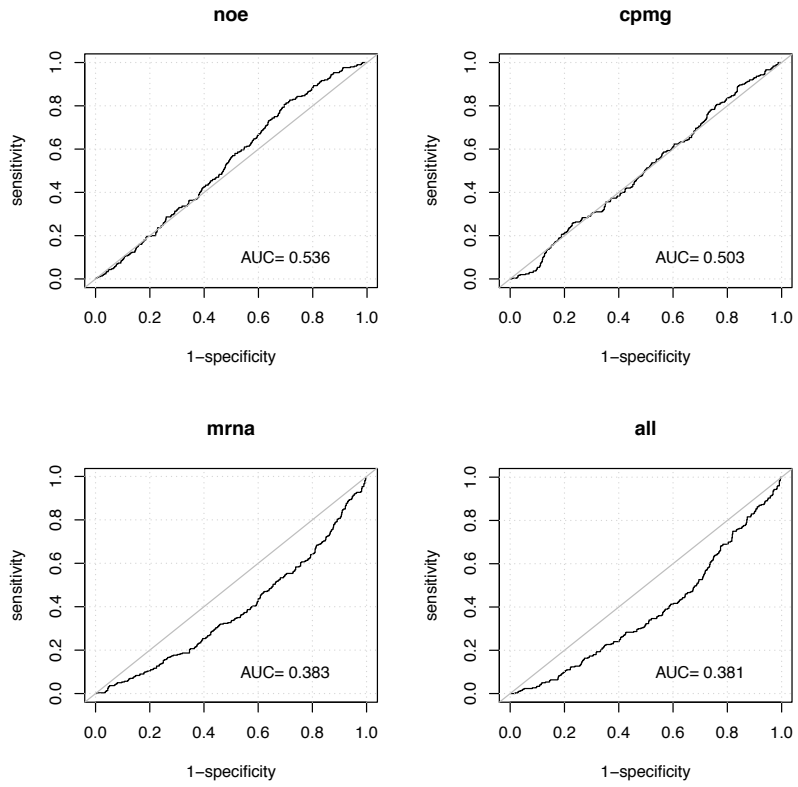

Figure 5: Prediction (logistic regression fitted by lasso) performance for "Duration" analysis. ROC curves for each data set.

	Name	HGNC	Ppm	Data set	Selection freq.
1894	ENSG00000077092_at	RARB		mrna	0.18
18953	ENSG00000245025_at			mrna	0.16
1374	ENSG00000061337_at	LZTS1		mrna	0.11

Table 17: selected variables (Duration, combined data set)

	Name	HGNC	Selection freq.
1330	ENSG00000077092_at	RARB	0.32
17923	ENSG00000235728_at		0.12
14704	ENSG00000186340_at	THBS2	0.11

Table 18: selected variables (Duration, mrna data set)

	Name	Ppm	Selection freq.
108		3.688078694	0.61
104		3.347534709	0.57
10	valine	0.976784495	0.54
123		3.799400243	0.5
168	glucose	4.629347879	0.47
135		4.005477649	0.45
80		2.828531781	0.44
114		3.726480719	0.43
96	pc	3.214817528	0.41
45		2.165289332	0.39
97	gpc	3.225218334	0.3
26	acetate	1.91089789	0.29
98		3.239711261	0.29
124		3.804976661	0.29
122		3.782266901	0.28
146		4.16221968	0.28
162		4.477803679	0.27
90	creatine	3.024960251	0.25
129		3.936503585	0.24
103	scyllo-inositol	3.335121944	0.22
212		8.344651987	0.22
173	glycogen	5.403066701	0.19
5		0.932254863	0.18
85	aspargine	2.956200282	0.17
113		3.719207131	0.17
154		4.336956988	0.17
81		2.907385432	0.16
210		8.223479012	0.15
83	aspargine	2.932435158	0.14
112		3.712430882	0.13
46		2.178066051	0.12
73		2.657284529	0.12
120		3.762413489	0.12
1	lipid	0.88249657	0.11
59	glutamine	2.423782982	0.11
148		4.22639782	0.11

175	glycogen	5.414940797	0.11

Table 19: selected variables (Duration, noe data set)

	Name	Ppm	Selection freq.
277		4.767992875	0.75
48		1.97267515	0.65
310	tyrosine	6.874495023	0.36
199		3.727119949	0.35
156		3.092754442	0.34
309	fumarate	6.509836489	0.31
191		3.68024848	0.29
266		4.48200363	0.28
10	valine	0.976657294	0.27
212		3.792718617	0.26
257		4.332907817	0.23
172	pc	3.215948458	0.2
192		3.689158497	0.18
183	scyllo-inositol	3.334861322	0.17
274		4.652478622	0.17
202		3.742516185	0.16
333		8.026599627	0.15
179		3.296905	0.14
288		5.784504915	0.14
17		1.062044033	0.13
231		4.013974573	0.13
298		5.963174077	0.13
180		3.315476883	0.12
111	glutathione	2.567515644	0.11
167		3.170412542	0.11
211		3.787352757	0.11

Table 20: selected variables (Duration, cpmg data set)

1.6 DebutLess25

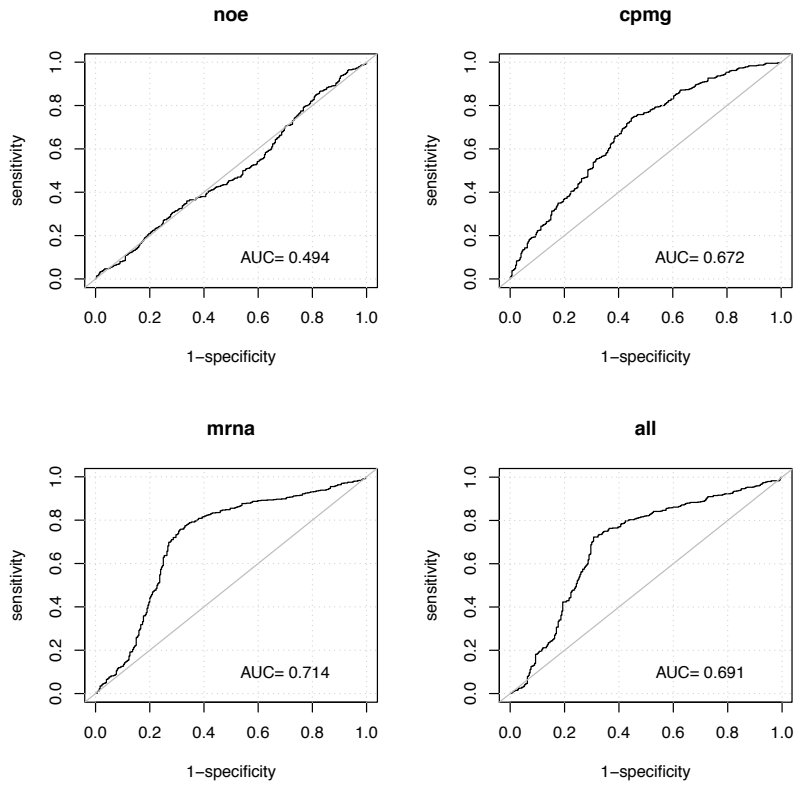

Figure 6: Prediction (logistic regression fitted by lasso) performance for "DebutLess25" analysis. ROC curves for each data set.

	Name	HGNC	Ppm	Data set	Selection freq.
15201	ENSG00000185942_at	NKAIN3		mrna	0.96
17900	ENSG00000229196_at			mrna	0.37
16956	ENSG00000206177_at	HBM		mrna	0.25
12615	ENSG00000170178_at	HOXD12		mrna	0.19
319			7.362883464	cpmg	0.15
1771	ENSG00000073754_at	CD5L		mrna	0.15
4937	ENSG00000116151_at	MORN1		mrna	0.14
5564	ENSG00000121764_at	HCRTR1		mrna	0.13
6368	ENSG00000128596_at	CCDC136		mrna	0.11
8424	ENSG00000142233_at	NTN5		mrna	0.11

Table 21: selected variables (DebutLess25, combined data set)

	Name	HGNC	Selection freq.
14637	ENSG00000185942_at	NKAIN3	0.98
17336	ENSG00000229196_at		0.28
16392	ENSG00000206177_at	HBM	0.21
1207	ENSG00000073754_at	CD5L	0.19
7860	ENSG00000142233_at	NTN5	0.17
5000	ENSG00000121764_at	HCRTR1	0.16
19330	ENSG00000259650_at		0.14
9065	ENSG00000152348_at	ATG10	0.13
12051	ENSG00000170178_at	HOXD12	0.13
9293	ENSG00000154478_at	GPR26	0.12

Table 22: selected variables (DebutLess25, mrna data set)

	Name	Ppm	Selection freq.
130		3.942403273	0.67
47		2.196867564	0.41
209		8.214158014	0.34
103	scyllo-inositol	3.335121944	0.33
85	aspargine	2.956200282	0.32
115		3.732386624	0.32
136		4.012266332	0.32
174	glycogen	5.409612677	0.32
18	lactate	1.332269992	0.3
48	lipid	2.253171801	0.26
93		3.185916927	0.26
214		8.599450426	0.26
169	glucose	4.64544428	0.24
194	tyrosine	7.168431479	0.21
49		2.299844441	0.2
144		4.124154567	0.2
140	myo-inositol	4.053887421	0.19
75		2.687719603	0.18
50		2.313179481	0.17
129		3.936503585	0.16
211		8.253616906	0.16

99		3.246531461	0.15
94	choline	3.197767026	0.12
95		3.206803792	0.12
64	glutathione	2.541030977	0.11
70		2.618800798	0.11
145		4.134580044	0.11

Table 23: selected variables (DebutLess25, noe data set)

	Name	Ppm	Selection freq.
252		4.26315663	0.83
262		4.409154783	0.8
276		4.758837295	0.63
319		7.362883464	0.61
274		4.652478622	0.58
169		3.188072049	0.54
315		7.257793947	0.4
22	lactate	1.332504019	0.35
40		1.742570797	0.33
4	isoleucine	0.92261137	0.3
105		2.521715744	0.27
200		3.732820994	0.26
136		2.892594136	0.24
257		4.332907817	0.23
198		3.721555455	0.22
279		5.169145106	0.2
335		8.202448906	0.18
114		2.618684459	0.15
209		3.776751919	0.15
230		4.009875576	0.15
159		3.112153115	0.12
231		4.013974573	0.12
255		4.28480121	0.12
108	glutathione	2.547507381	0.11
184		3.346628064	0.11
296		5.935568788	0.11

Table 24: selected variables (DebutLess25, cpmg data set)

2 Prediction results (OPLS-DA)

2.1 ActiveControl

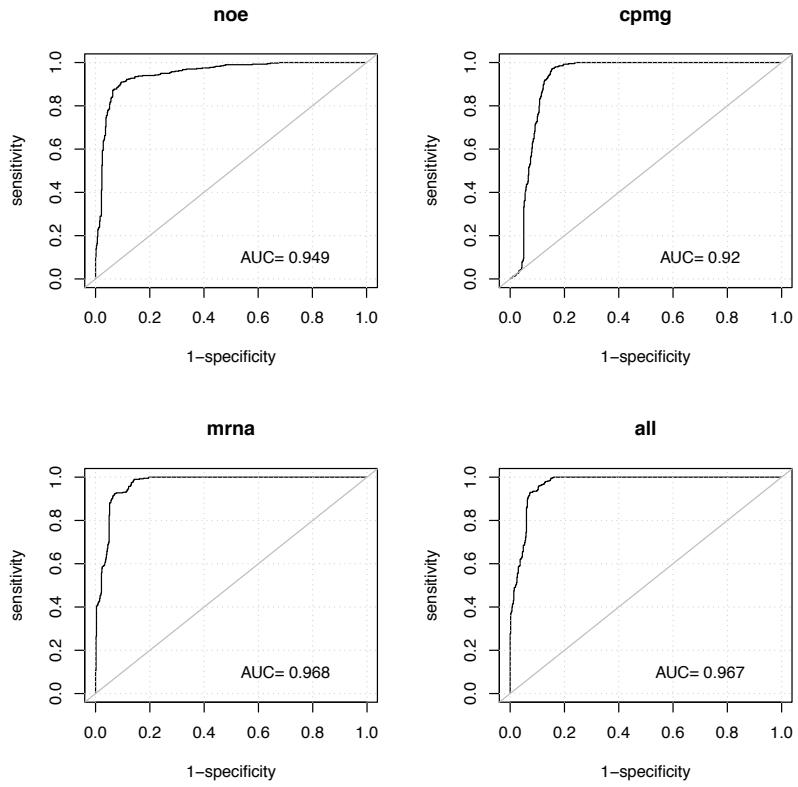

Figure 7: Prediction (OPLS) performance for "activeControl" analysis. ROC curves for each data set.

2.2 InactiveActive

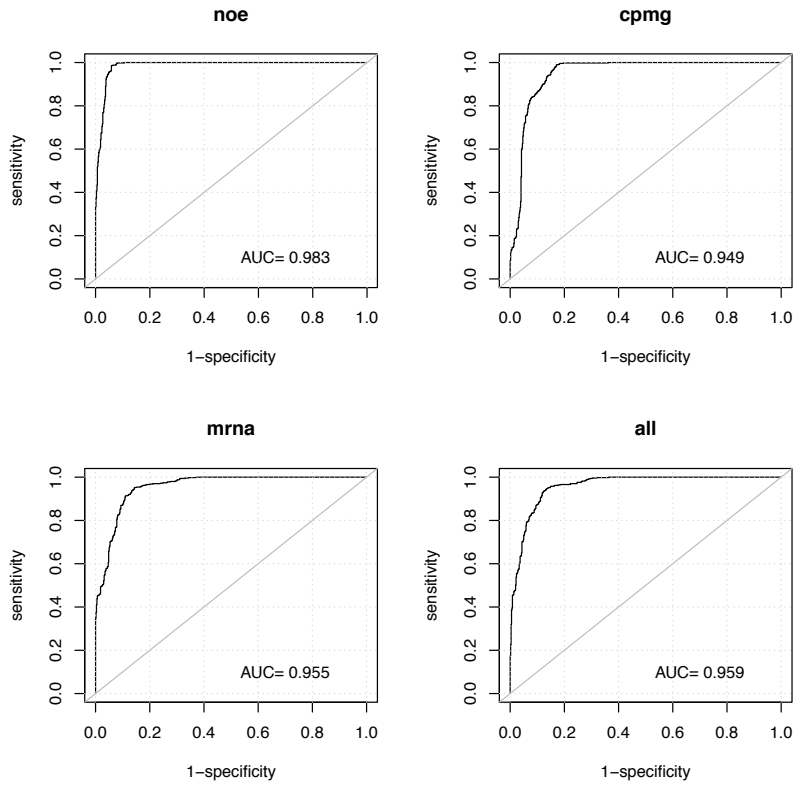

Figure 8: Prediction (OPLS) performance for "InactiveActive" analysis. ROC curves for each data set.

2.3 InactiveControl

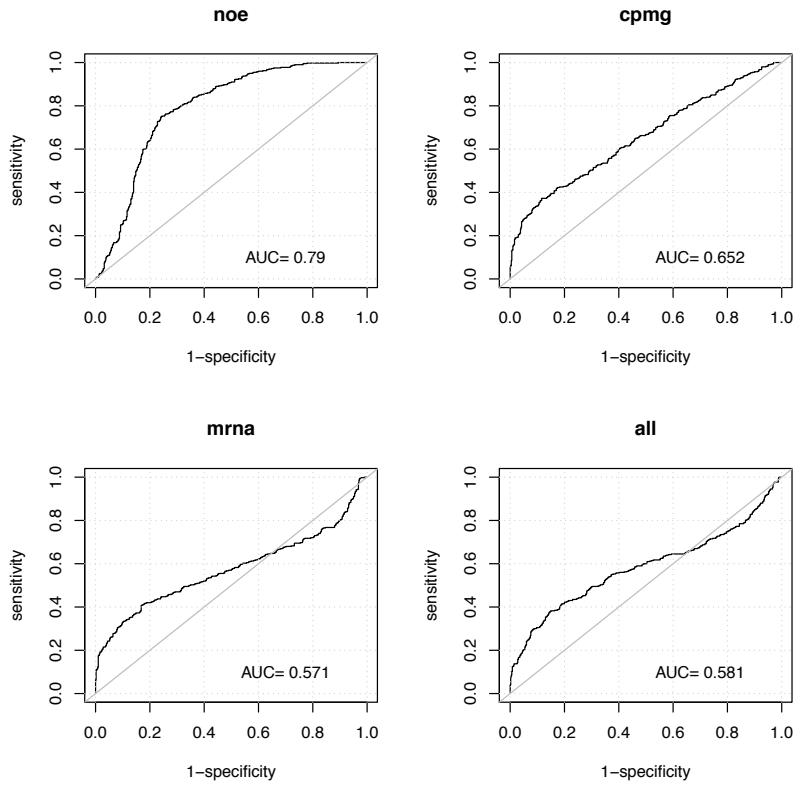

Figure 9: Prediction (OPLS) performance for "InactiveControl" analysis. ROC curves for each data set.

2.4 SiSd

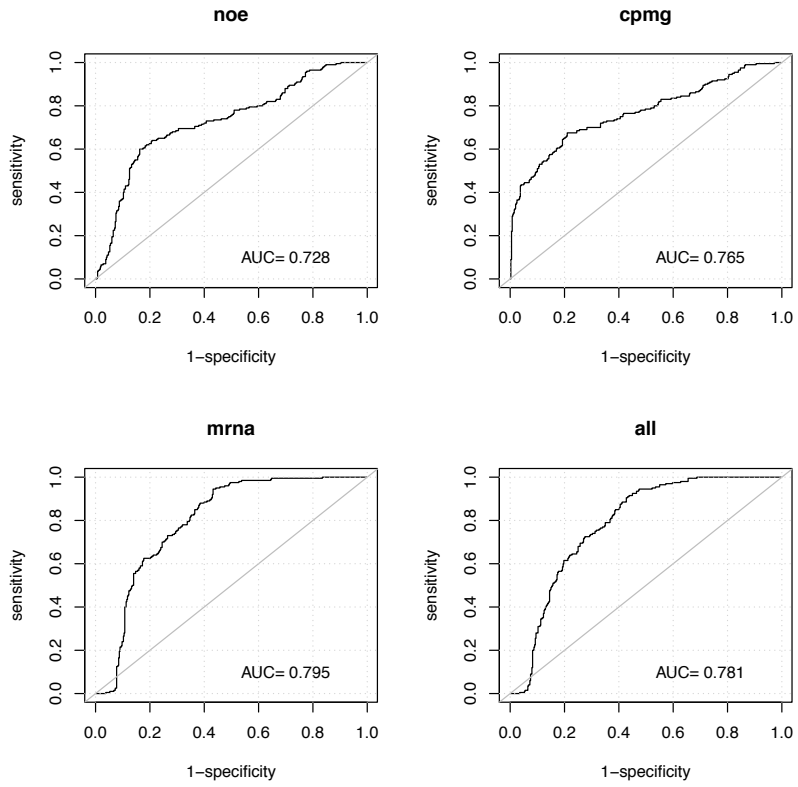

Figure 10: Prediction (OPLS) performance for "SiSd" analysis. ROC curves for each data set.

2.5 DebutLess25

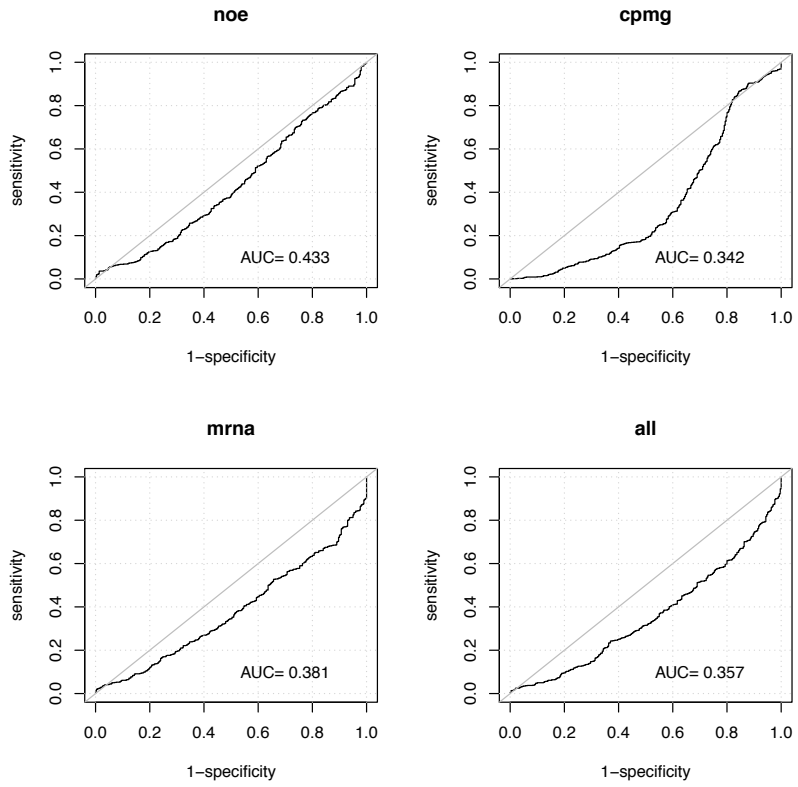

Figure 11: Prediction (OPLS) performance for "DebutLess25" analysis. ROC curves for each data set.

2.6 Duration

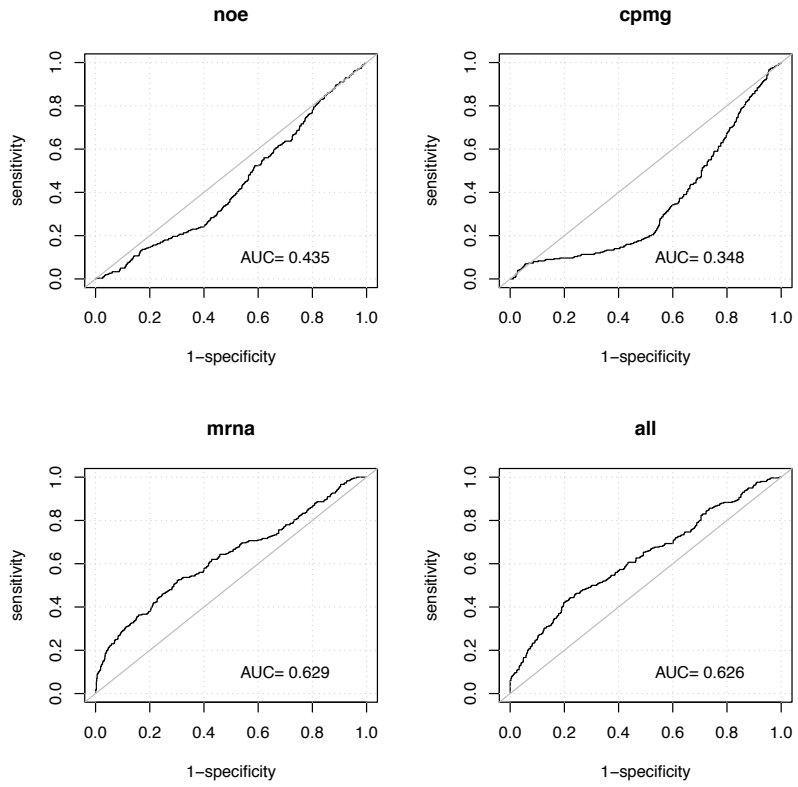

Figure 12: Prediction (OPLS) performance for "Duration" analysis. ROC curves for each data set.