

Table 3.

Best classifiers without isomirs			
molecular features	n	NPV	PPV
TSC.TSC2 + hsa.miR.21.5p + thymine	62	0.958	0.921
ENSG00000213025 + ENSG00000224796 + ENSG00000254859	65	0.759	0.962
TSC.TSC2 + Q13740 + ENSG00000231419	64	0.861	0.918
TSC.TSC2 + hsa.miR.130a.3p + ENSG00000214776	60	--	0.944
ENSG00000213025 + ENSG00000224796 + carnitine	63	0.811	0.927
TSC.TSC2 + hsa.miR.21.5p + acadesine	62	0.941	0.896
TSC.TSC2 + hsa.miR.769.5p + thymine	62	0.799	0.928
Q08380 + ENSG00000267046 + ENSG00000227135	64	0.837	0.915
TSC.TSC2 + glycine + thymine	66	0.819	0.922
TSC.TSC2 + Q13740 + ENSG00000214776	64	0.804	0.922
Best classifiers with isomirs			
ENSG00000237693 + carnitine + hsa.miR.584.5p_T_3prime_TTATGGTTTGCCTGGGACTGAGT	41	0.997	1.000
TSC.TSC2 + ENSG00000214776 + hsa.miR.92a.3p_CG_3prime_TATTGCACTTGTCCCGGCCTGTCTG	42	0.987	1.000
TSC.TSC2 + ENSG00000214776 + hsa.miR.329.3p_trim2_AACACACCTGGTTAACCTCT	42	0.967	1.000
TSC.TSC2 + Q13740 + hsa.miR.144.3p_A_3prime_TACAGTATAGATGATGTACTA	44	0.982	0.996
ENSG00000227135 + hsa.miR.548e.3p_trim1_AAAACTGAGACTACTTTTGC hsa.miR.485.3p_trim2_GTCATACACGGCTCTCCTCT	42	0.958	1.000
TSC.TSC2 + ENSG00000214776 + hsa.miR.500a.3p_A_5prime_AATGCACCTGGGCAAGGATTCTG	42	0.973	0.996
TSC.TSC2 + ENSG00000214776 + hsa.miR.323a.3p_G_5prime_GCACATTACACGGTCGACCTCT	42	0.978	0.994

ENSG00000227135	+	42	0.952	0.997
hsa.miR.548e.3p_trim1_AAAAACTGAGACTACTTTTGC	+			
hsa.miR.410.3p_trim3_AATATAACACAGATGGCC				
ENSG00000237693	+	42	0.939	0.999
hsa.miR.548e.3p_trim1_AAAAACTGAGACTACTTTTGC	+			
hsa.miR.584.5p_T_3prime_TTATGGTTTGCCTGGGACTGAGT				
P04217	+	44	0.957	0.995
hsa.miR.323a.3p_G_5prime_GCACATTACACGGTCGACCTCT	+			
hsa.miR.582.5p_trim1_TTACAGTTGTTCAACCAGTTAC				

Notes: TSC.TSC2 refers to mutation in TSC2; hsa.miR refers to an miR species; ENSG refers to an mRNA; Q refers to a protein group assessed by mass spec; metabolites are given by name.