





Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 28 putative biomarkers.

Metric	1-ad	2-ad	3-ad	1-rd	2-rd	3-rd	2-cr	3-cr	2-sd	3-sd
Sens	61.1	65.2	65.9	61.1	69.1	67.7	66.7	65.8	66.7	67.9
Spec	60.0	73.3	75.3	58.6	64.4	73.0	65.5	72.2	65.5	69.7
%Undet	0.0	0.6	3.9	1.7	14.4	28.9	6.7	13.9	6.7	14.4
Quality	121.1	137.9	137.3	118.1	119.1	111.8	125.5	124.1	125.5	123.2

Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 28 putative biomarkers with the caveat that %Undetermined cannot exceed 5.0%.

Metric	1-ad	2-ad	3-ad	1-rd	2-rd	3-rd	2-cr	3-cr	2-sd	3-sd
Sens	61.1	65.2	65.9	61.1	None	None	59.3	None	59.3	None
Spec	60.0	73.3	75.3	58.6	None	None	65.9	None	66.7	None
%Undet	0.0	0.6	3.9	1.7	None	None	3.3	None	3.3	None
Quality	121.1	137.9	137.3	118.1	None	None	121.9	None	122.1	None

## Fingerprint Analysis

Sensitivity, specificity and quality (sensitivity + specificity) for the best and 200<sup>th</sup> best decision tree constructed from any of the 300 peak intensities. The evolutionary programming search used a population size of 200 and ran for 400 generations. A decision node became a terminal node when it contained 1% (no samples) or 4% (3 samples) of a given State.

Metric	1%		1%		4%		4%	
	1 <sup>st</sup>	200 <sup>th</sup>						
Sensitivity	83.3	85.6	87.8	83.3	71.1	72.2	87.8	87.8
Specificity	76.7	73.3	74.4	76.7	88.9	74.4	72.2	70.0
Quality	160.0	158.9	162.2	160.0	160.0	156.7	160.0	157.8

Sensitivity, specificity and quality (sensitivity + specificity) for the best and 200<sup>th</sup> best medoid classifier algorithm in each of the two runs using 5-, 6-, and 7-peak intensities from the set of 300. The evolutionary programming search used a population size of 400 and ran for 800 generations with the requirement that there are at most 60 Case-cells and 60 Control-cells.

Metric	5-Features		5-Features		6-Features		6-Features		7-Features		7-Features	
	1 <sup>st</sup>	200 <sup>th</sup>										
Sens	100.0	100.0	85.6	77.8	100.0	100.0	87.8	81.1	100.0	100.0	90.0	82.2
Spec	83.3	78.9	100.0	100.0	86.7	81.1	100.0	100.0	88.9	82.2	100.0	100.0
Quality	183.3	178.9	185.6	177.8	186.7	181.1	187.8	181.1	188.9	182.2	190.0	182.2

(Last updated 4/21/07)