





Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 26 putative biomarkers.

Metric	1-ad	2-ad	3-ad	1-rd	2-rd	3-rd	2-cr	3-cr	2-sd	3-sd
Sens	57.3	58.7	63.0	57.0	58.7	61.6	60.6	61.6	60.6	62.5
Spec	58.3	59.0	58.1	58.1	58.7	60.5	54.7	58.5	55.0	58.4
%Undet	0.0	0.0	0.8	0.3	5.2	45.0	0.8	9.8	0.8	9.3
Quality	115.7	117.7	120.2	114.7	112.2	99.7	114.5	110.3	114.8	111.5

Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 26 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	57.3	58.7	63.0	57.0	58.7	None	60.6	None	60.6	None
Spec	58.3	59.0	58.1	58.1	54.6	None	54.7	None	55.0	None
%Undet	0.0	0.0	0.8	0.3	4.7	None	0.8	None	0.8	None
Quality	115.7	117.7	120.2	114.7	108.6	None	114.5	None	114.8	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 400 and ran for 800 generations. A decision node became a terminal node when it contained 1% (3 samples) or 4% (12 samples) of a given State.

Metric	1%		1%		4%		4%	
	1 <sup>st</sup>	200 <sup>th</sup>						
Sensitivity	75.7	71.0	64.0	63.0	70.3	74.0	79.3	79.3
Specificity	62.7	66.3	72.3	72.3	67.0	62.0	56.3	55.3
Quality	138.3	137.3	136.3	135.3	137.3	136.0	135.7	134.7

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 1000 and ran for 2000 generations with the requirement that there are at most 200 Case-cells and 200 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	70.3	63.3	100.0	100.0	75.7	72.3	100.0	100.0	78.7	75.0
Spec	67.3	63.3	100.0	100.0	76.3	71.7	100.0	100.0	79.7	75.0	100.0	100.0
Quality	167.3	163.3	170.3	163.3	176.3	171.7	175.7	172.3	179.7	175.0	178.7	175.0

(Last updated 4/21/07)