





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	65.0	65.0	75.0	64.4	70.8	76.7	75.0	70.6	76.5	70.0
Spec	68.3	75.0	78.8	68.4	77.4	79.5	71.4	81.6	71.4	81.6
%Undet	0.0	0.0	13.3	3.3	15.8	27.5	10.0	16.7	10.8	17.5
Quality	133.3	140.0	140.5	129.5	132.4	128.8	136.4	135.6	137.1	134.1

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	65.0	65.0	70.0	64.4	None	None	66.1	None	66.1	None
Spec	68.3	75.0	64.4	68.4	None	None	61.7	None	61.7	None
%Undet	0.0	0.0	0.8	3.3	None	None	3.3	None	3.3	None
Quality	133.3	140.0	133.6	129.5	None	None	124.4	None	124.4	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% (2 samples) of a given State.

Metric	1%		1%		4%		4%	
	1 <sup>st</sup>	200 <sup>th</sup>						
Sensitivity	83.3	83.3	93.3	90.0	88.3	86.7	85.0	81.7
Specificity	88.3	88.3	85.0	85.0	88.3	86.7	88.3	90.0
Quality	171.7	171.7	178.3	175.0	176.7	173.3	173.3	171.7

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 400 and ran for 800 generations with the requirement that there are at most 40 Case-cells and 40 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	93.3	83.3	100.0	100.0	93.3	86.7	100.0	100.0	93.3	88.3
Spec	90.0	83.3	100.0	100.0	91.7	85.0	100.0	100.0	93.3	86.7	100.0	100.0
Quality	190.0	183.3	193.3	183.3	191.7	185.0	193.3	186.7	193.3	186.7	193.3	188.3

(Last updated 4/21/07)