





Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 31 putative biomarkers.

Metric	1-ad	2-ad	3-ad	1-rd	2-rd	3-rd	2-cr	3-cr	2-sd	3-sd
Sens	54.0	63.2	65.6	54.2	64.9	58.5	61.5	61.6	61.4	60.5
Spec	56.7	58.2	56.9	57.4	53.8	61.9	58.9	59.5	57.9	60.3
%Undet	0.0	0.3	0.3	0.8	7.2	20.7	0.3	11.3	0.5	11.2
Quality	110.7	121.1	122.1	110.8	111.5	99.8	120.1	109.7	118.8	109.7

Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 31 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	54.0	63.2	65.6	54.2	56.4	None	61.5	None	61.4	None
Spec	56.7	58.2	56.9	57.4	53.4	None	58.9	None	57.9	None
%Undet	0.0	0.3	0.3	0.8	5.0	None	0.3	None	0.5	None
Quality	110.7	121.1	122.1	110.8	104.8	None	120.1	None	118.8	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>	1 <sup>st</sup>	200 <sup>th</sup>	1 <sup>st</sup>	200 <sup>th</sup>	1 <sup>st</sup>	200 <sup>th</sup>
Sensitivity	67.0	67.7	67.7	66.3	72.7	71.3	76.3	70.7
Specificity	70.0	68.3	68.7	69.0	64.3	64.3	61.3	65.7
Quality	137.0	136.0	136.3	135.0	137.0	135.7	137.7	136.3

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>	1 <sup>st</sup>	200 <sup>th</sup>	1 <sup>st</sup>	200 <sup>th</sup>	1 <sup>st</sup>	200 <sup>th</sup>	1 <sup>st</sup>	200 <sup>th</sup>	1 <sup>st</sup>	200 <sup>th</sup>
Sens	100.0	100.0	69.3	63.3	100.0	100.0	79.0	72.7	100.0	100.0	80.3	75.7
Spec	69.7	63.3	100.0	100.0	75.3	71.3	100.0	100.0	78.7	74.0	100.0	100.0
Quality	169.7	163.3	169.3	163.3	175.3	171.3	179.0	172.7	178.7	174.0	180.3	175.7

(Last updated 4/21/07)