

Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 22 putative biomarkers.

Metric	1-ad	2-ad	3-ad	1-rd	2-rd	3-rd	2-cr	3-cr	2-sd	3-sd
Sens	76.7	74.1	80.8	76.7	65.4	77.3	80.8	90.0	76.9	90.0
Spec	72.4	77.8	77.8	69.0	86.4	90.9	76.9	82.1	77.8	85.2
%Undet	1.7	10.0	11.7	1.7	20.0	26.7	13.3	20.0	11.7	21.7
Quality	147.4	141.9	146.9	144.0	131.7	141.5	144.4	152.1	143.0	153.5

Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 22 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	76.7	69.0	71.4	76.7	None	None	72.4	None	72.4	None
Spec	72.4	70.0	79.3	69.0	None	None	64.3	None	64.3	None
%Undet	1.7	1.7	5.0	1.7	None	None	5.0	None	5.0	None
Quality	147.4	137.3	145.7	144.0	None	None	131.7	None	131.7	None

Fingerprint Analysis

Sensitivity, specificity and quality (sensitivity + specificity) for the best and 200th 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% (1 sample) of a given State.

Metric	1%		1%		4%		4%	
	1 st	200 th	1 st	200 th	1 st	200 th	1 st	200 th
Sensitivity	96.7	96.7	93.3	90.0	96.7	93.3	100.0	100.0
Specificity	93.3	93.3	100.0	100.0	100.0	100.0	96.7	93.3
Quality	190.0	190.0	193.3	190.0	196.7	193.3	196.7	193.3

Sensitivity, specificity and quality (sensitivity + specificity) for the best and 200th 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 20 Case-cells and 20 Control-cells.

Metric	5-Features		5-Features		6-Features		6-Features		7-Features		7-Features	
	1 st	200 th	1 st	200 th	1 st	200 th	1 st	200 th	1 st	200 th	1 st	200 th
Sens	100.0	100.0	100.0	93.3	100.0	100.0	100.0	100.0	100.0	100.0	100.0	96.7
Spec	100.0	90.0	100.0	100.0	100.0	96.7	100.0	100.0	100.0	100.0	100.0	100.0
Quality	200.0	190.0	200.0	193.3	200.0	196.7	200.0	200.0	200.0	200.0	200.0	196.7

(Last updated 4/21/07)